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CR 85-01

ASSESSMENT OF THE PERFORMANCE OF AN IN-FIELD GAUSSIAN PLUME/PUFF MODEL FOR OVERWATER USE

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A U.S. Navy chemical hazard forecast computer model is tested for consistency with Naval Postgraduate School field data which was used in its development. The model's attempt to forecast puff dispersion, for which a parameterization has not been developed, are examined by comparison to relative dispersion data sets. The parameterizations developed from the NPS data set are compared to an independently derived set of parameterizations demonstrating the generic applicability of the model. It was found that the model predicts the total width over which a hazard might occur reasonably well, but underpredicts the downwind hazard distance. This is due to lack of separate consideration of meander effects.

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CONTENTS

I. INTRODUCTION

The U.S. Navy is currently in the process of developing a capability to forecast chemical weapons hazard (CWH) for the overwater regime. This is part of the Shipboard Numerical Aids Program (SNAP). The present implementation of CWH is encoded in the BASIC programming language, and is designed for use on the HP9845B micro-computer.

Among the major goals during the development of CWH for SNAP were speed, user-friendly operation, easy to interpret results, and flexibility. The program runs extremely quickly, typically producing the graphics output within about 10 seconds (neglecting time for user inputs). This is accomplished in part by using the relatively simple analytical Gaussian plume formula as the core, and in part by efficient programming techniques. The program is easily operated by a computer novice, with default options available for all user inputs. Since the program is designed to be operational from shipboard during a potential battle situation, the output is configured in easy to interpret polar coordinates with radial compass bearing spokes spreading out from the contaminant source, and "danger zones" contoured in units representing hazard to human life. The program is written using meaningful variable names and a modular format. This will facilitate easy modifications and additions in the future.

The purpose of the herein described research was to investigate the behavior of the model under a full spectrum of meteorological conditions, comparing predicted results to

measured values. As a first step, those measured values were the same data used to parameterize the Gaussian model. On first thought, this procedure should be a needless, redundant exercise. We will see, however, that this is not the case since some valuable insights into model performance are brought forth.

Next, the model results were tested against a "pseudo-instantaneous" data set to examine how the model treats burst, or puff, releases. As puff releases are of major concern in the application of SNAP, these results are very important to the model validation study.

Finally, the model equations were compared to results of a recent tracer experiment in the North Sea to test their applicability at different locations. The true test of any such model is its geographic independence.

II. METHODOLOGY

In order to compare the model output to measured values, the basic model equations must be presented and discussed. The familiar Gaussian plume dispersion model, for a surface release with no vertical limit to the plume spread is based on the equation:

$$C(x,y,z) = \frac{S}{\pi \sigma_y \sigma_z U} \exp\left[- \frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2}\right] , \qquad (1)$$

where $C(x,y,z)$ is concentration, mass/volume

- S is the source emission rate, mass/time
- x,y,z are distances measured from the release point origin
- U is the mean wind speed (in the x direction)
- $\sigma_y(x)$ is the standard deviation of the plume's horizontal mass distribution
- $\sigma_z(x)$ is the standard deviation of the plume's vertical mass distribution

Note that σy and σz are functions of downwind distance, x, due to plume spread. The factor S/U in the equation takes into account that the material released in time dt is spread over length Udt. We have assumed 100% reflection of the plume at the ground.

Obtaining the biological effects due to the plume is a simple matter since Equ 1 predicts a nonchanging concentration at each point in space. This concentration can be used to calculate a dose rate, the total dose for some time period, etc. simply by determining the total amount of air involved.

The situation is not so simple for an instantaneous release of material, a burst, because the concentration at a point in space is a time changing quantity. Equ 1 is also used for this case, with the source emission rate replaced by total amount of material released and the calculated quantity being "dosage" rather than concentration. In order to understand the comparison of this equation, as used in CWH model, to the simulated burst data it is necessary to understand how it is obtained.

For a burst, the concentration is given by

$$C = 2\,\frac{Q}{(2\pi)^{3/2}\sigma_{x'}\sigma_y\sigma_z}\,\exp\left[-\frac{x'^2}{2\sigma_{x'}^2}-\frac{y^2}{2\sigma_y^2}-\frac{z^2}{2\sigma_z^2}\right], \tag{2}$$

where Q is the total amount of material released and the factor of 2 multiplier accounts for ground reflection. In Equ 2, x' is measured from the center of mass of the puff; we suppress the time dependence of the concentration for the sake of simplicity. The time dependence of the location of the center of mass can be simply introduced using the mean wind speed.

We can define the dose at some point in space as the total amount of material that crosses a given area aligned perpendicular to the mean wind as the puff advects past the point. Dose is given by

$$\text{dose} = \Delta y\Delta z\,\frac{Q}{\pi\sigma_y\sigma_z}\,\exp\left[-\frac{y^2}{2\sigma_y^2}-\frac{z^2}{2\sigma_z^2}\right], \tag{3}$$

where $\Delta y\Delta z$ is the area. In what follows we will use a unit area, $\Delta y\Delta z = 1$. Equ 3 is obtained by integrating Equ 2 over all x. The standard deviations are functions of the distance from the release

point, as in Equ 1. Note that dose depends only on the parameters which describe the puff.

For biological applications, it is important to know how long a particular level of concentration remains at a point, rather than the total dose. For this reason the quantity dosage is introduced. We assume that the mean wind speed does not contribute to the spread of the puff other than how it affects the turbulence spectrum. The only affect of the speed is to transport the puff at a particular rate. Thus, the length of time that the calculated concentration will exist at a point depends inversely on the wind speed. Dosage is defined to be the dose divided by the wind speed:

$$D = \text{dose}/60U, \tag{4}$$

where we have used the factor of 60 to change the units from kg sec/m^3 to kg min/m^3, the common usage for calculating hazards to personnel.

The CWH model calculates ground level, hazard isopleths. The isopleths are the loci of coordinates for a particular predetermined dosage. We let the specified dosage be D_s, and the value of crosswind distance at which this dosage occurs for some downwind distance be y_s. Then, using the definition of dosage given in Equ 4, substituting Equ 3 for dose, and setting z=0, for ground level impact, we easily derive:

$$y_s(x) = \sigma_y\left[2\ln(Q/60\pi D_s\sigma_y\sigma_z U)\right] \tag{5}$$

The maximum downwind distance at which this dosage can occur can be found by setting y=0 and solving for x. Since the x-dependence is absorbed in the standard deviations, it is necessary to have analytical forms for these quantities before this step can be carried out. This is done by parameterizing puff growth using experimental data; the results are presented in Skupniewicz and Schacher (1984).

The forms needed are:

$$\sigma_y(x) = ax^c$$
$$\sigma_z(x) = bx^d \tag{6}$$

The values of the constants, a, b, c, d, can be found in the reference. Substituting in Equ 5 for the standard deviations, substituting y=0, and solving for x gives:

$$x_{max} = (q/60D_s abU)^{(1/(c+d))} \tag{7}$$

The CWH model computes lethality isopleths that are referenced to the expected percent of personnel that will be casualties. For example, LD50-GD means that the specified dosage would result in 50% casualties from the gas GD. In order to convert the Gaussian calculation of dosage, which is based on the ambient concentration in the air, to lethality, it is necessary to know such quantities as inhalation rate, biological effects, etc. The CWH model contains the information needed to make the conversion in a look-up table, which is based on the total mass reaching the lungs in 1 min.

The experimental data which are used for this model validation study come from tracer measurements of ambient concentration, mass

per unit volume, from a continuous release plume. As can be seen from what has been presented above, all that is needed to convert the source rates to mass released, in order to simulate a burst release, is to multiply the rate by 1 min, 60 sec. This converts individual surface concentration measurements to dosage for direct comparison to the CWH model isopleths. Since the CWH model graphics output is in units of lethal dosage, we have also had to use the model's look-up table to convert experimentally determined dosages to those units. Once this was done, we had transects of lethal dosage as a function of crosswind distance for various downwind distances. The experimental transects are far enough apart in time and space that they cannot be used to construct isopleths. Rather, we compare the CWH model results to the individual transects. This was done by superimposing, on the model output, the location of the center of the plume, and by using hashmarks connected by a line through the center point to indicate the locations where the concentration falls to the value appropriate to the specified lethality. The results are shown in the next section.

III. COMPARISON TO ONE-HOUR AVERAGED CONCENTRATION PROFILES

These results use, as a data base, a subset of the data used to produce the sigma-y and sigma-z parameterizations implemented in CWH. Only data whose ground-level concentration transects were known, or could be derived, were selected. Also, only those data whose absolute coordinates were known (in relation to the source and mean wind direction) were used. By applying these criteria and forming hourly averages of the experimental data, direct comparison to CWH output could be made.

As with the original sigma formulae, the data were divided into Pasquill-Gifford equivalent stability classes. For an explanation of the techniques involved in the sigma parameterizations and the determination of stability class over water, see Schacher, et. al. (1982). In addition, data within each stability class were binned into wind speed categories with a range of 2 m/s each.

Figures 1.1-1.12 present the CWH model isopleths and the hourly averaged composite transects, starting with the most stable (E), lowest wind speed case and progressing through the least stable (B), highest wind speed case. The representation of the transect data is explained in the former section. A single plotted transect is the average of 2 to 15 instantaneous "snapshots" of the continuous plume.

The CWH output has an "N" that indicates north. Note that the model graphics uses both 0 and 360 for the north bearing, and

also uses ± angles when 0 is used for north. No reason for these two presentations is known.

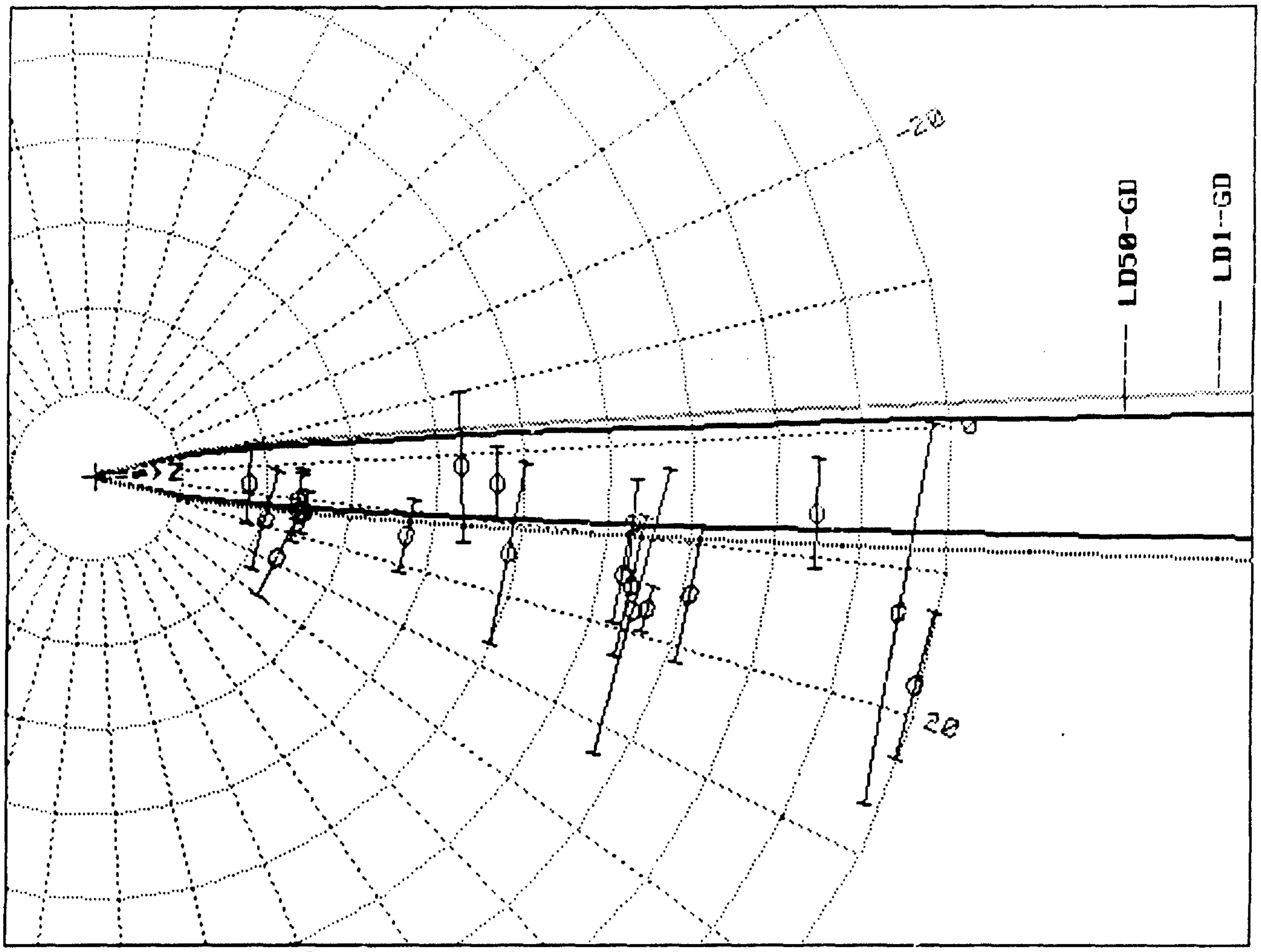
The stability/windspeed categories have varying numbers of transects, and not all windspeed categories have entries. Classes B and C contain only a small number of transects and conclusions based on these data cannot be drawn.

Figure 1. SNAP one-minute dosage output for various NPS stability classes and windspeed categories compared to hourly averaged concentration transects. Open circles locate the center of mass. Hash marks correspond to LD1-GD . The model's source size and lethal dosage levels have been scaled down to match the experimental release rates. Note that ring scaling occasionally changes from 1000 to 500 yards. An arrow at the source indicates true north. The following table gives wind speed and class for each figure.

FIGURE	NPS/P-G STABILITY CLASS	WINDSPEED
1.1	E	3-4 m/s
1.2	E	4-5
1.3	D	2-3
1.4	D	3-4
1.5	D	4-5
1.6	D	5-6
1.7	D	6-7
1.8	D	7-8
1.9	D	8-9
1.10	D	over 9
1.11	C	4-5
1.12	B	2-3

Fig. 1.1

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS　　BEARINGS IN DEG TRUE　　PLOT FORMAT #1

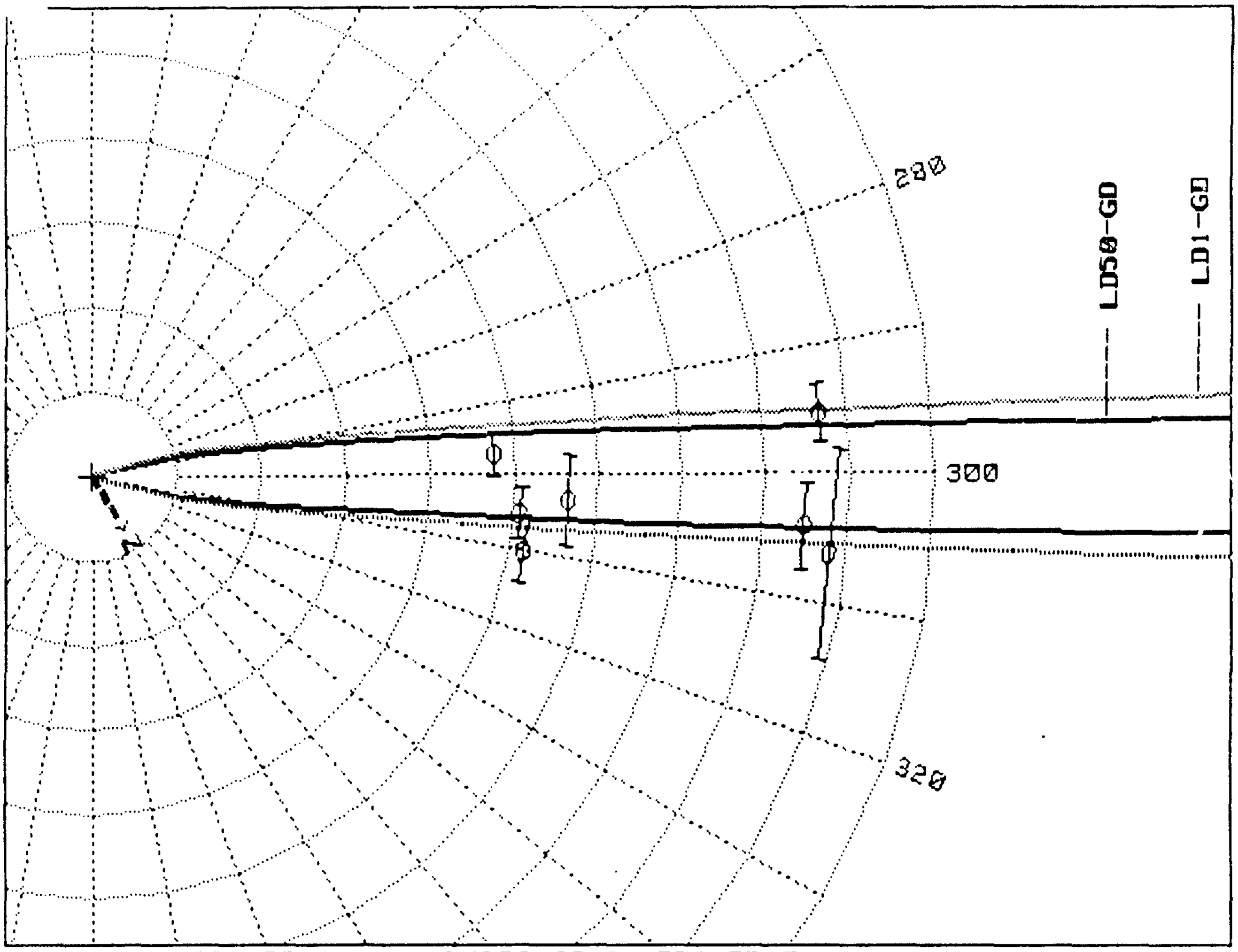
TERRAIN TYPE	OPEN-SEA
MEAN WIND	7.77000777001 KTS　FROM 183.44047619 DEG TRUE
STABILITY CATAGORY	E　MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	43316 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	129039 YARDS

FOR TEST AND EVALUATION USE ONLY!

Fig. 1.2

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	9.71250971251 KTS FROM 120.222222222 DEG TRUE
STABILITY CATAGORY	E MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

===

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	36337 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	108246 YARDS

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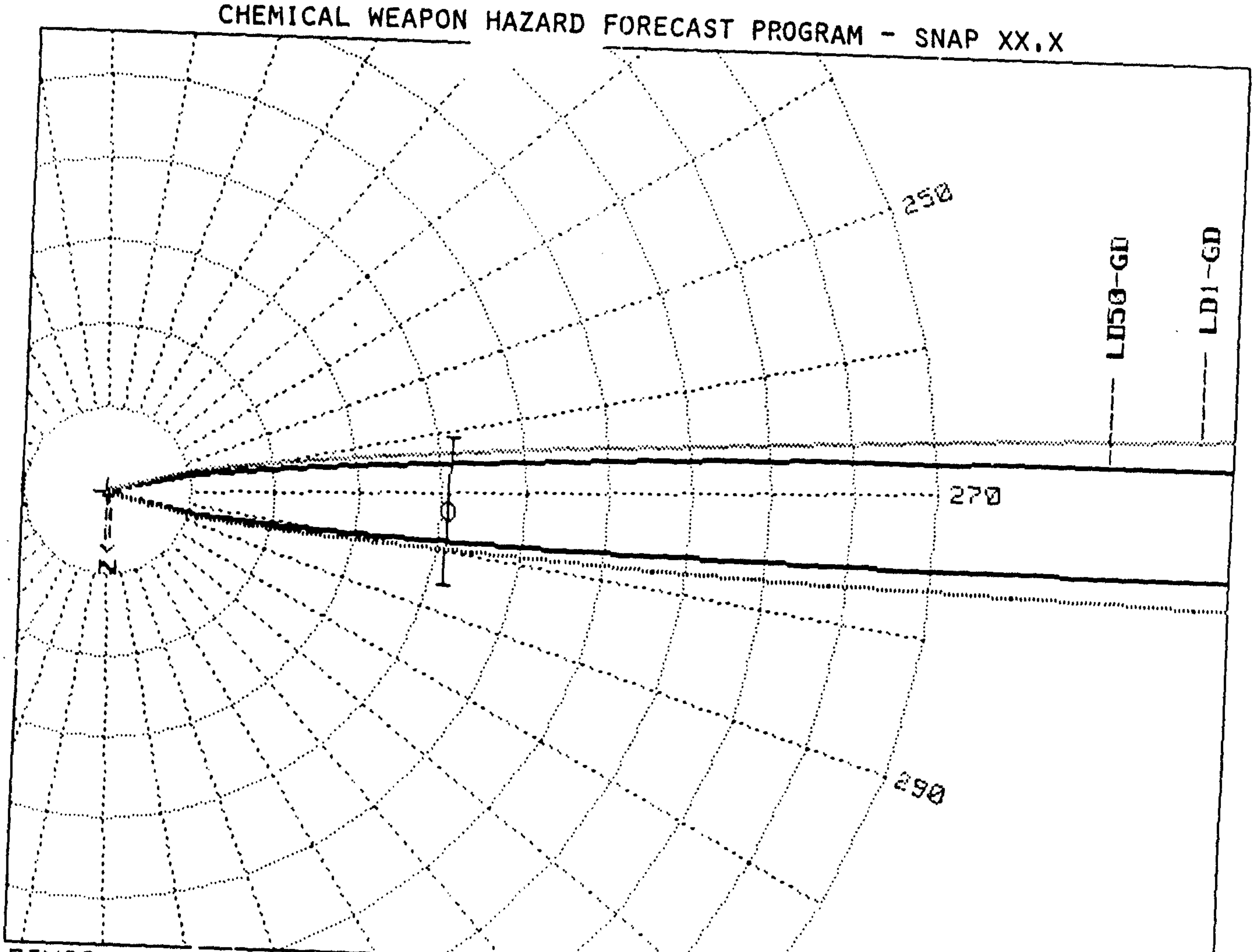
Fig. 1.3

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS BEARINGS IN DEG TRUE PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	5.82750582751 KTS FROM 91.6333333333 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	26109 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	73468 YARDS

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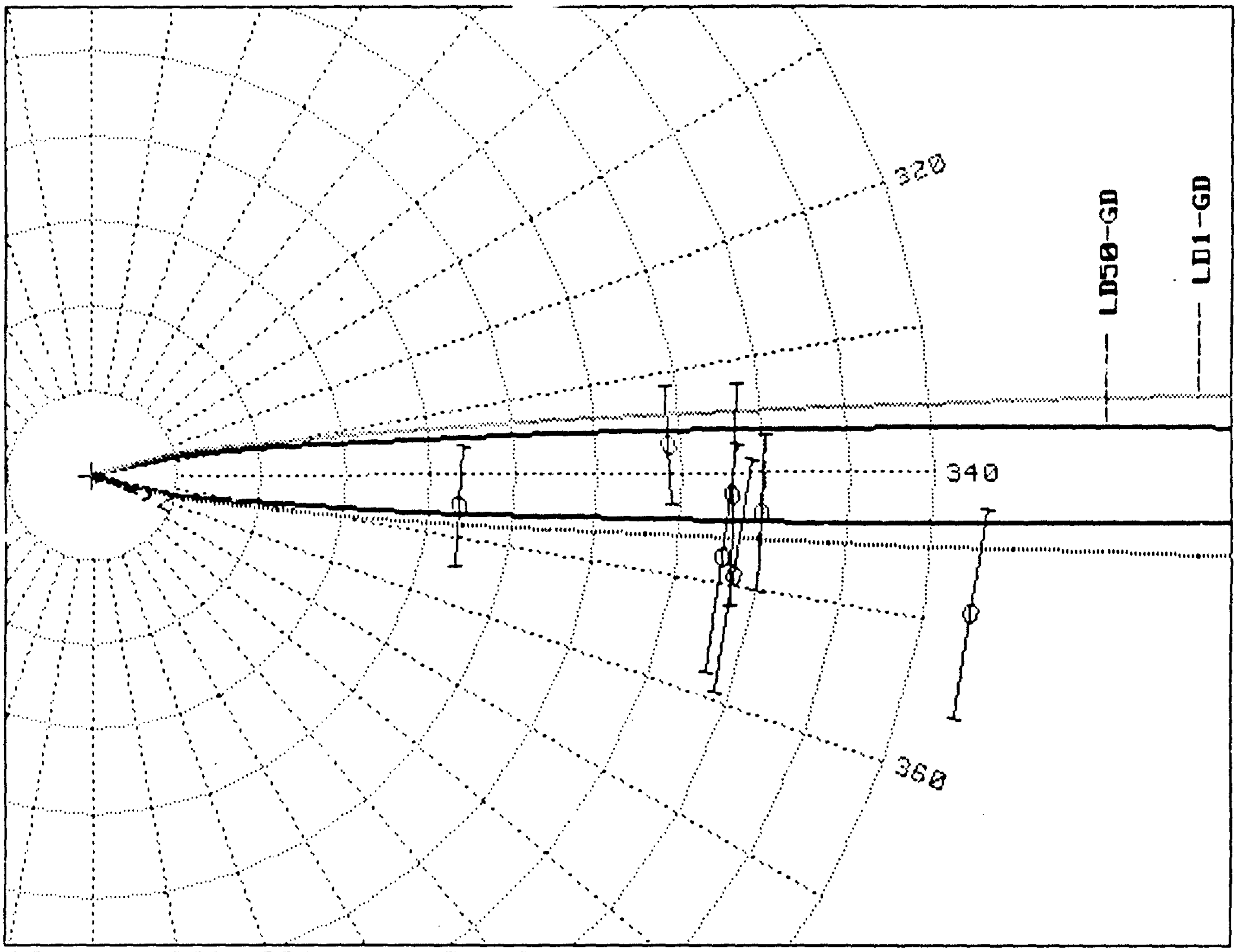
Fig. 1.4

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS BEARINGS IN DEG TRUE PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	7.77000777001 KTS FROM 160.2 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

===

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	21065 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	59274 YARDS

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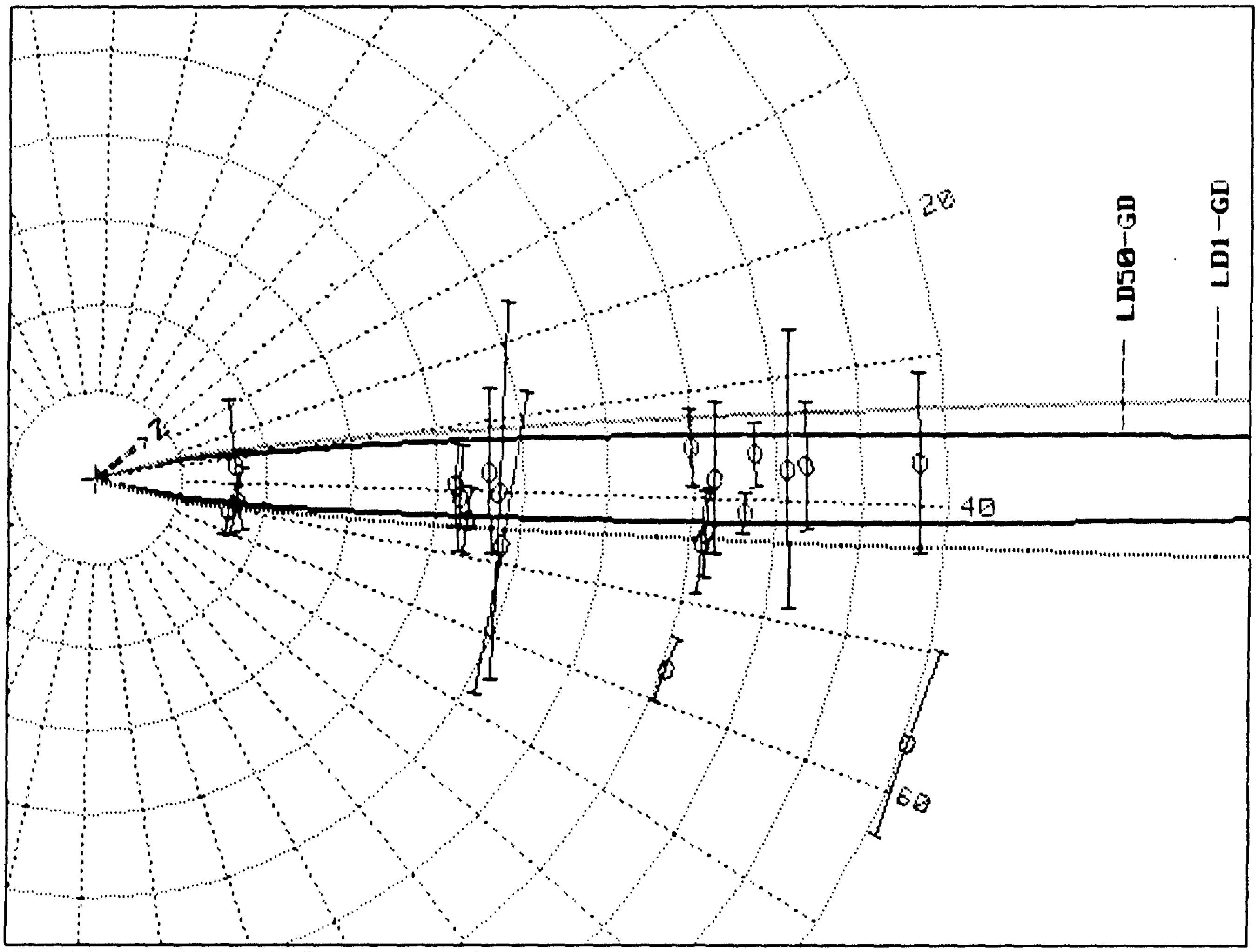
Fig. 1.5

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	9.71250971251 KTS FROM 219.190909091 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	17833 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	50181 YARDS

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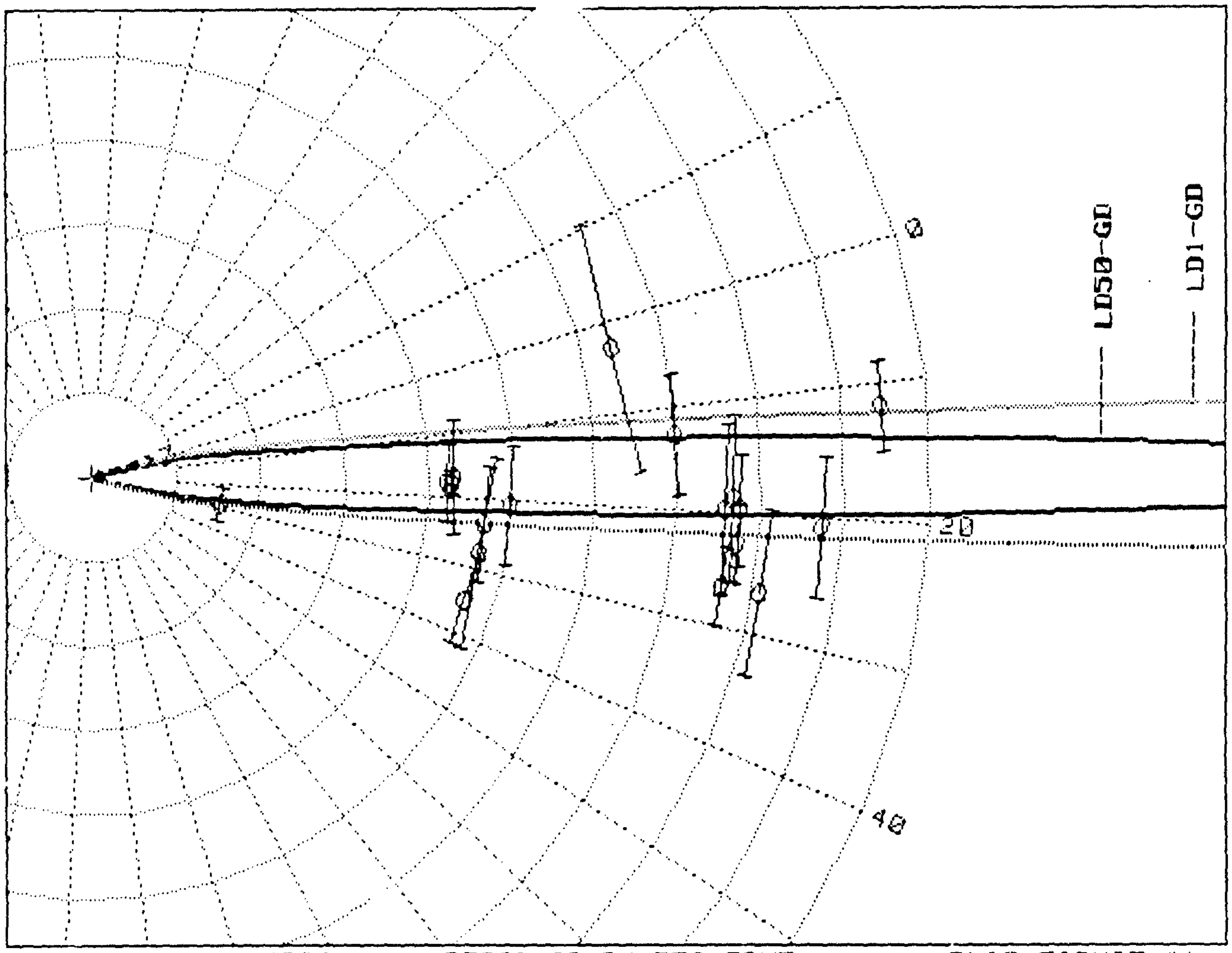
Fig. 1.6

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS　　BEARINGS IN DEG TRUE　　PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	11.655011655 KTS FROM 196.615 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	15565 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	43798 YARDS

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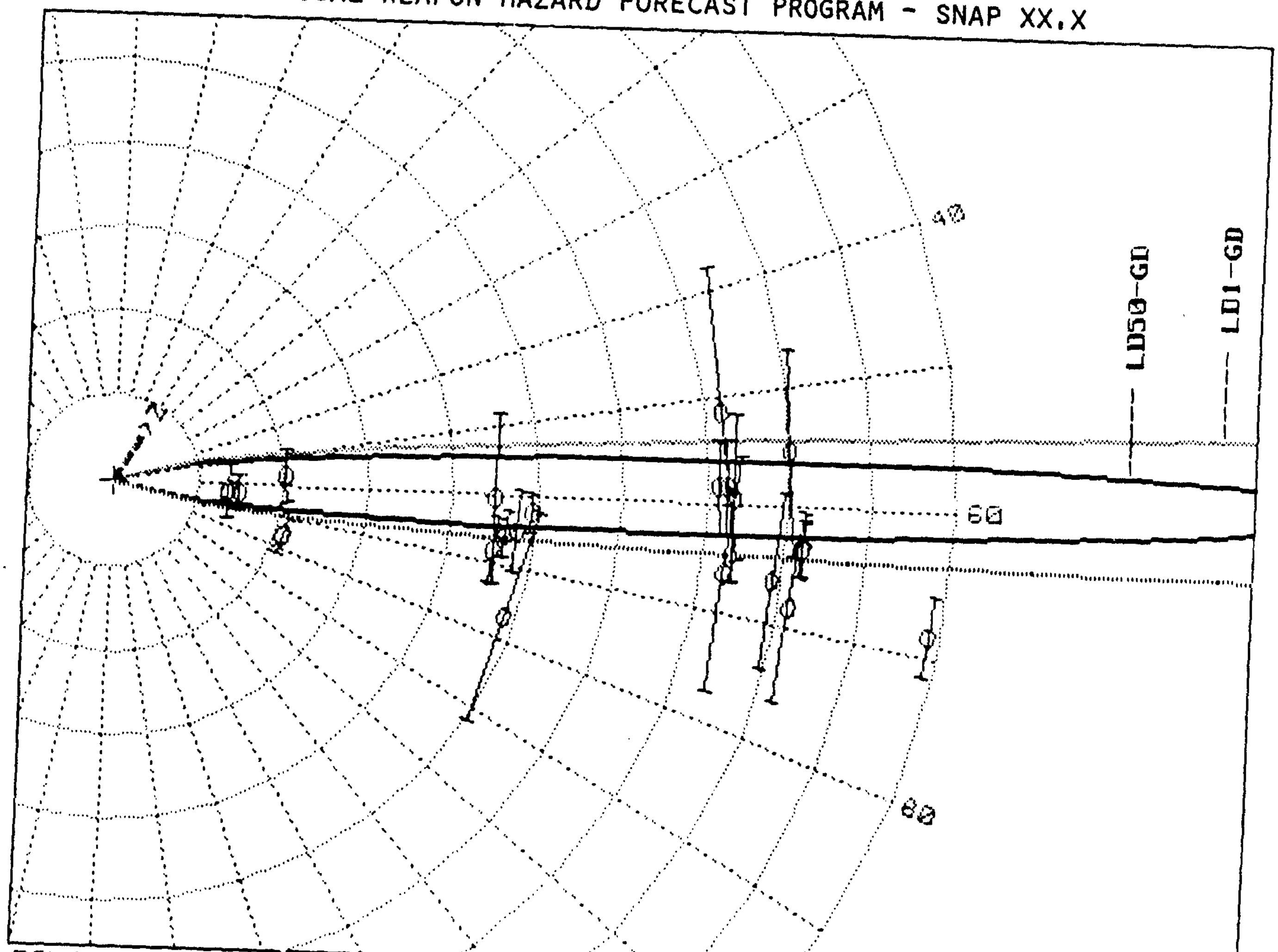
Fig. 1.7

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA		
MEAN WIND	13.5975135975 KTS	FROM	239.416666667 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL		
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)		
SOURCE TYPE	POINT-BURST		
SOURCE SIZE (effective)	.189 KG		
SOURCE RATE	INSTANTANEOUS		

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	30% DEATHS - MOST INCAPACITATED	13873 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	39038 YARDS

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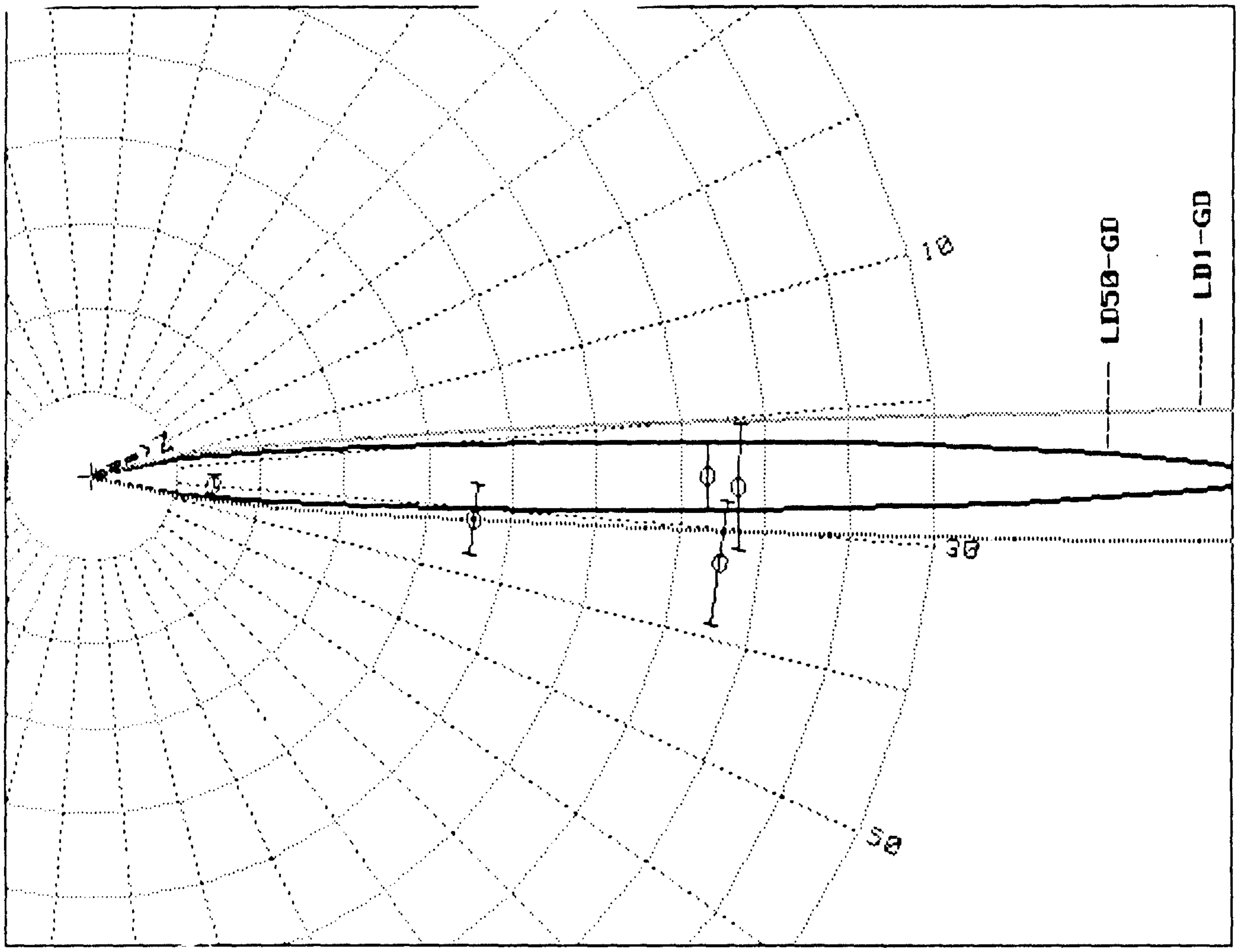
Fig. 1.8

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS BEARINGS IN DEG TRUE PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	15.54001554 KTS FROM 205.1285?1429 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	12557 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	35335 YARDS

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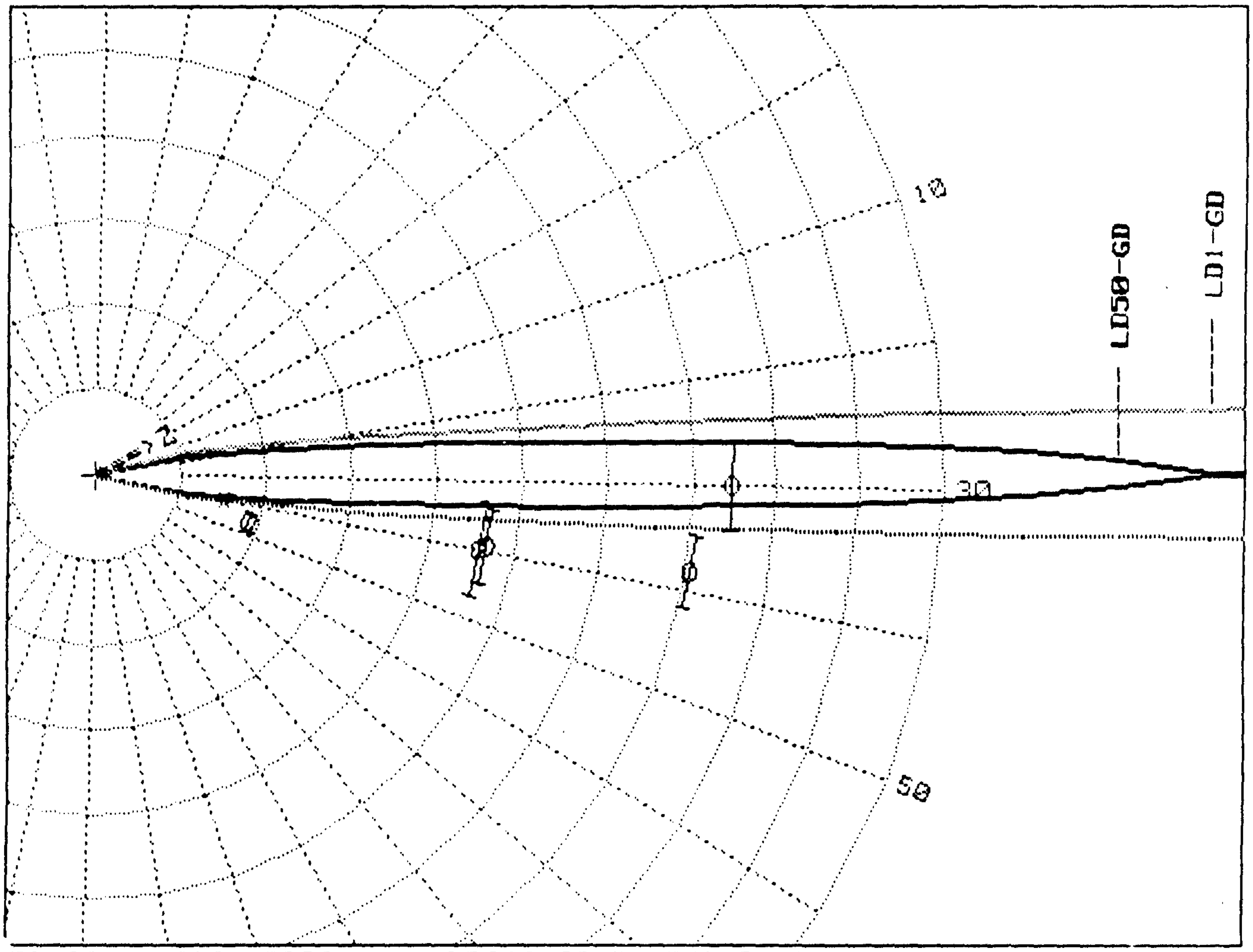
Fig. 1.9

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS BEARINGS IN DEG TRUE PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	17.4825174825 KTS FROM 208.94375 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	11501 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	32362 YARDS

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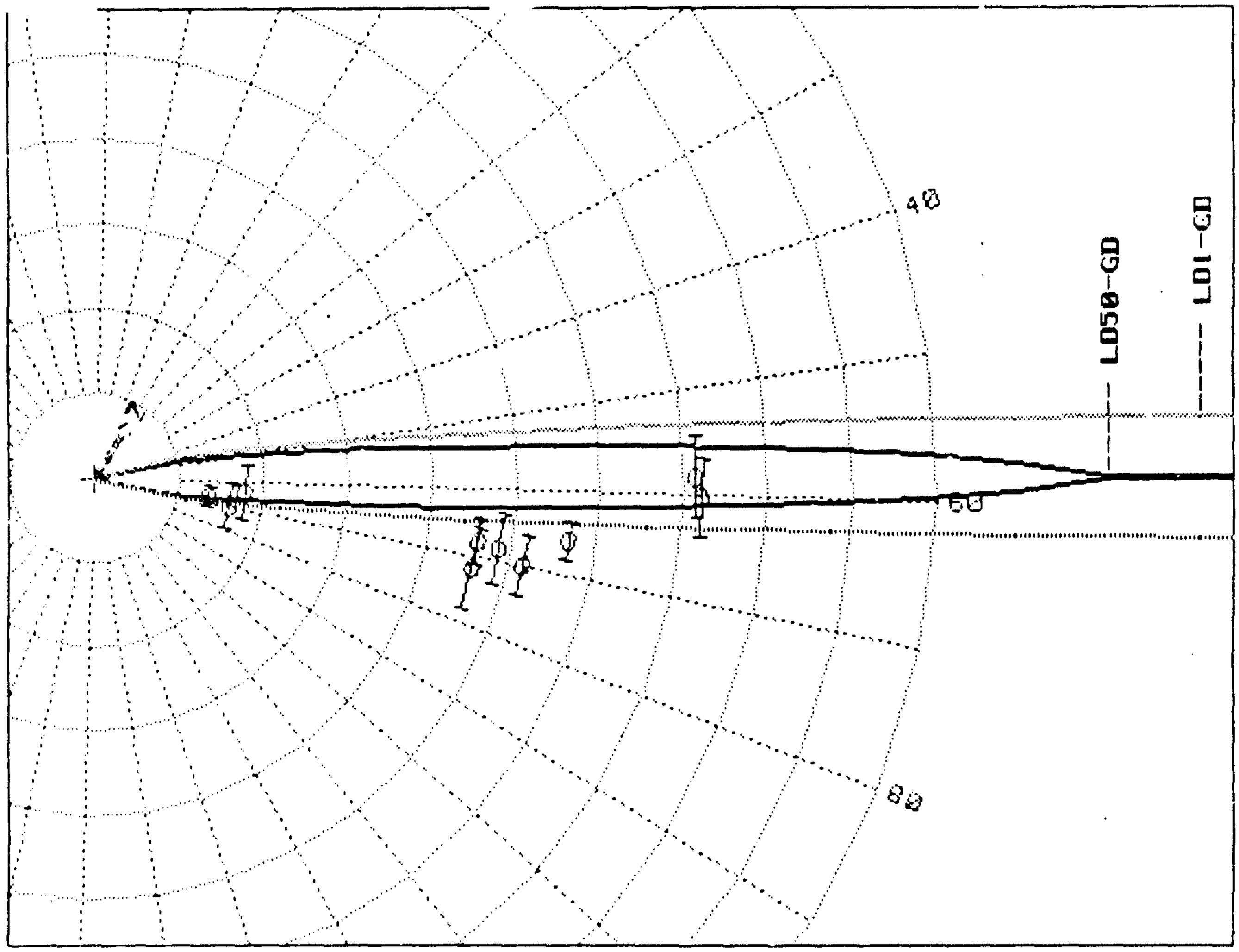
Fig. 1.10

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS BEARINGS IN DEG TRUE PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	19.425019425 KTS FROM 238.320833333 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	10631 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	29915 YARDS

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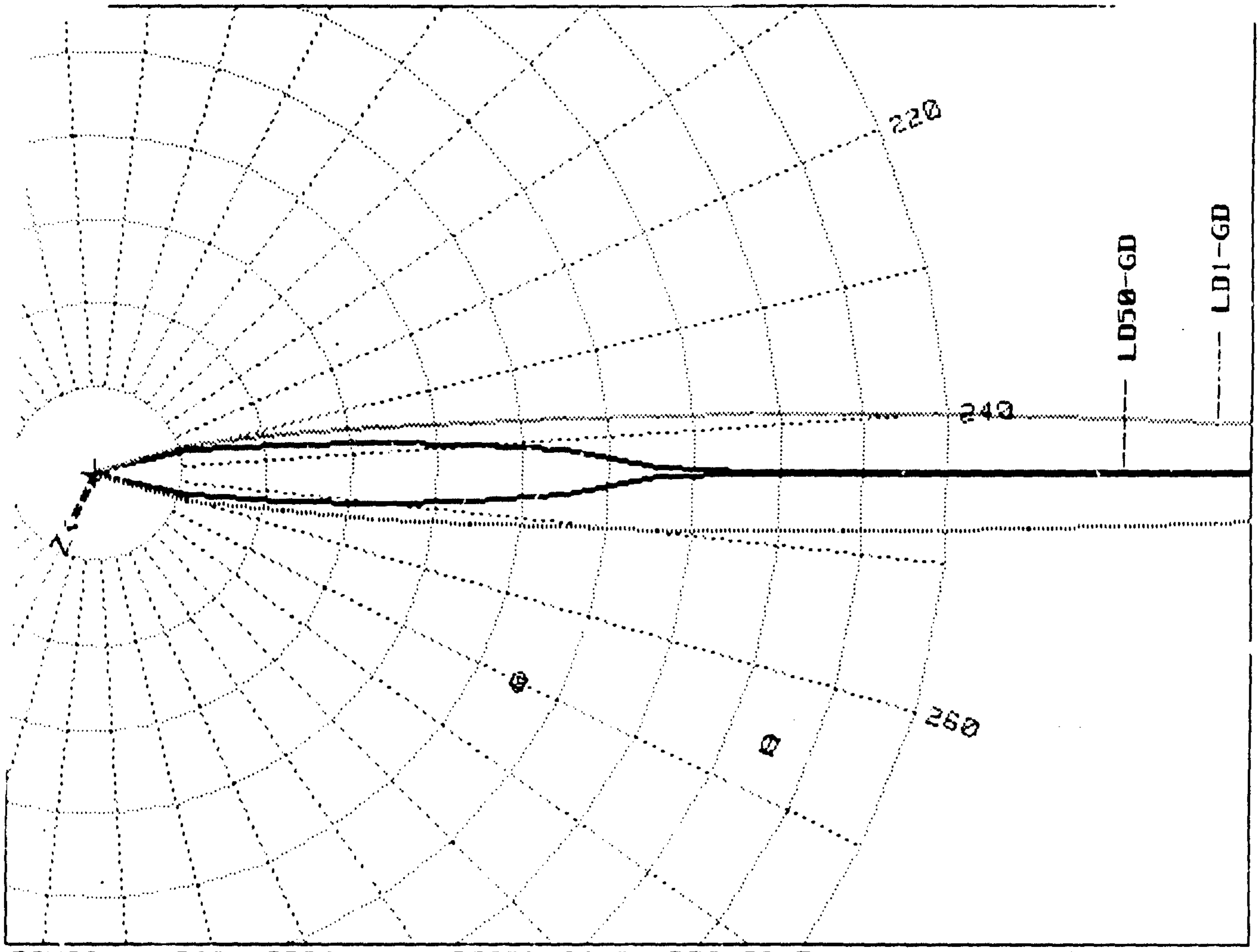
Fig. 1.11

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	9.71250971251 KTS FROM 64 DEG TRUE
STABILITY CATAGORY	C MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	6024 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	16216 YARDS

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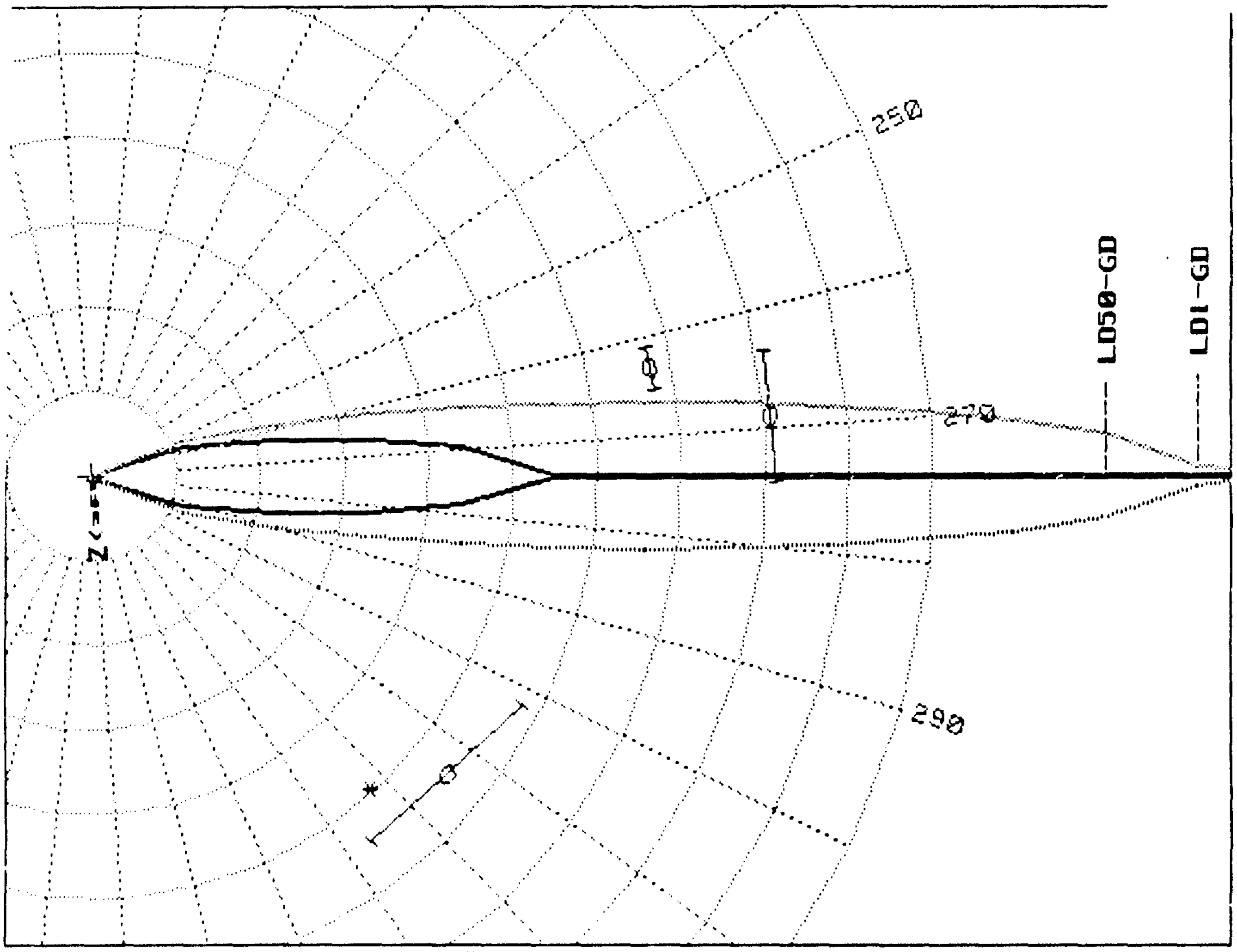
Fig. 1.12

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	5.82750582751 KTS FROM 94 DEG TRUE
STABILITY CATAGORY	B MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	4780 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	12045 YARDS

FOR TEST AND EVALUATION USE ONLY!

Examination of these plots immediately shows that the cloud does not consistently follow the mean flow, even with one hour averaging. Variation of the actual cloud size is quite large, typically ranging from 1/3 to 3 times the predicted size. These two facts tend to suggest that the predicted cloud size is underpredicted by CWH for a one-hour average of one-minute dosages (recall that CWH is predicting one-minute dosage of a single puff). It is obvious that meander effects (the scatter about the mean wind direction) should be included for a one-hour prediction.

CWH mathematically adjusts the puff "footprint" proportionally to ln(wind speed^{-1}). Examination of the wind speed categories, particularily class D, suggests that the actual footprint is affected by wind speed changes in a much more dramatic fashion. Most abnormally wide transects are associated with lower wind speed while the highest wind speed category exclusively contains transects narrower than the average.

This may be explained by the dependence of the surface roughness on wind speed over water. Roughness, and dispersion, will increase with increasing wind speed. As an example of how this may be important, consider class D. Class D, neutral, can result from either high wind speed or low air-sea temperature difference. Thus using a single class, with no explicit wind speed dependence, can not be adequate to describe diffusion. In addition, the effects of meander are damped with increasing wind speed. These effects suggest that the Pasquill-Gifford

stability classes do not sufficiently explain overwater dispersion and need refinement.

One obvious feature of most of the plots is the general tendency for the cloud to veer to the right with increasing range. This is a distinct characteristic of the sea-breeze regime, the dominant meso-scale synoptic situation during the tracer experiments. The mean wind was recorded at the release site, typically several miles offshore. As the sea breeze approaches the shoreline and the convergence zone, acceleration due to the pressure gradient decreases. The Coriolis force becomes more influential, "pulling" the flow to the right.

IV. COMPARISON TO PSEUDO-INSTANTANEOUS CONCENTRATION PROFILES

The primary goal of CWH, as stated earlier, is to predict total dosage realized over a one-minute period. Using one-hour average sigma formulae, as is presently implemented in CWH, will predict the average one-minute dosage experienced by releasing a statistically large number of puffs over a one-hour period. If the goal is to predict the impact of a single released puff, one-hour average sigma formulae will predict a wider and shorter region of impact than should be expected. This can be a conservative approach, from the user's point of view, in determining how far off the downwind axis is "safe", but dangerous when determining how far down the centerline axis is "safe". This will be explained more fully at the end of this section.

To examine the actual behavior of a single puff, a pseudo-instantaneous puff data set has been compiled. This set was produced by recombining the individual transects through the plume. The center of each transect was superimposed and new hourly averages formed. Such an average gives the "typical" cross-wind concentration dependence for a puff for that hour. Processing the data in this way removes meander from the results, so that the sigma-y produced contains only relative diffusion about the puff center of mass.

There are two assumptions made in this data analysis. Note that the data are obtained from measurements made during transects through a continuous plume, not a burst release. We assume that lateral and longitudinal dispersion are independent

when using a plume to simulate a burst. We further assume that the sizes of the plume and burst are approximately the same so that they would respond in the same way to the turbulence.

The results are shown in Figures 2.1-2.9. The size and placement of each "puff" is indicative of an individual puff. While these data are somewhat a function of averaging time, the individual profiles were measured over a short enough period of time so that, in most cases, the variance between individual transect's sigmas was small compared to the average size of the plume cross section (the pseudo-instantaneous cross section).

Examination of the figures reveals that the individual puff widths are almost exclusively less than or equal to the model prediction. This is convenient, in that the hourly average sigma values define the upper limit of puff growth for this data set. In addition, the area enveloped by CWH isopleths appear to be more representative of the scatter of puff profiles due to off-axis deviations of the centers of mass. This suggests that the "danger zone" predicted by CWH is representative of the total possible area of coverage by a burst rather than the area covered by a single burst.

In order to correctly interpret these results, it is important to recognize that the CWH model conserves mass. This means that, if it predicts too wide a hazard corridor, it must also predict too short a range for the hazard. This is almost a "conservation of area covered" principle. Comparison of the model predictions and the data shows that this is the way CWH behaves.

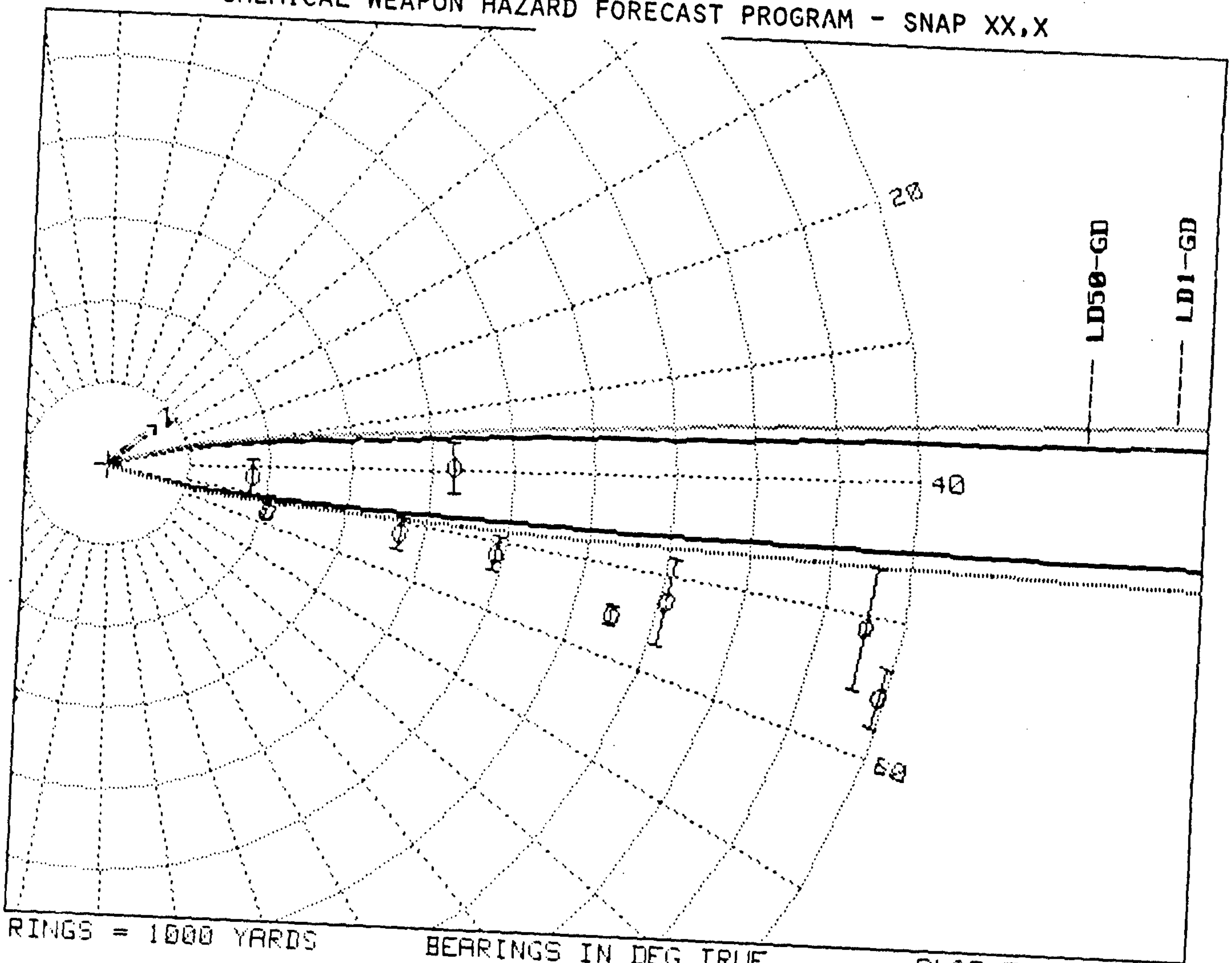
The data set used for these comparisons is not sufficiently large to enable separation of the relative diffusion about the center of mass and the meander, which would allow a true "scatter envelope" to be determined.

Figure 2. Same as Figure 1. except CWH output vs. pseudo-instantaneous averaged profiles. Note that this data set is significantly smaller than the hourly averaged data set (Figure 1). The following table gives windspeed and class for each figure.

FIGURE	NPS/P-G STABILITY CLASS	WINDSPEED
2.1	E	3-4
2.2	D	2-3
2.3	D	3-4
2.4	D	4-5
2.5	D	5-6
2.6	D	6-7
2.7	D	7-8
2.8	D	8-9
2.9	D	9+

Fig. 2.1

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX,X



RINGS = 1000 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA	
MEAN WIND	7.77000777001 KTS	FROM 221.113636364 DEG TRUE
STABILITY CATAGORY	E MODIFIED PASQUILL	
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)	
SOURCE TYPE	POINT-BURST	
SOURCE SIZE (effective)	.189 KG	
SOURCE RATE	INSTANTANEOUS	

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	43316 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	129039 YARDS

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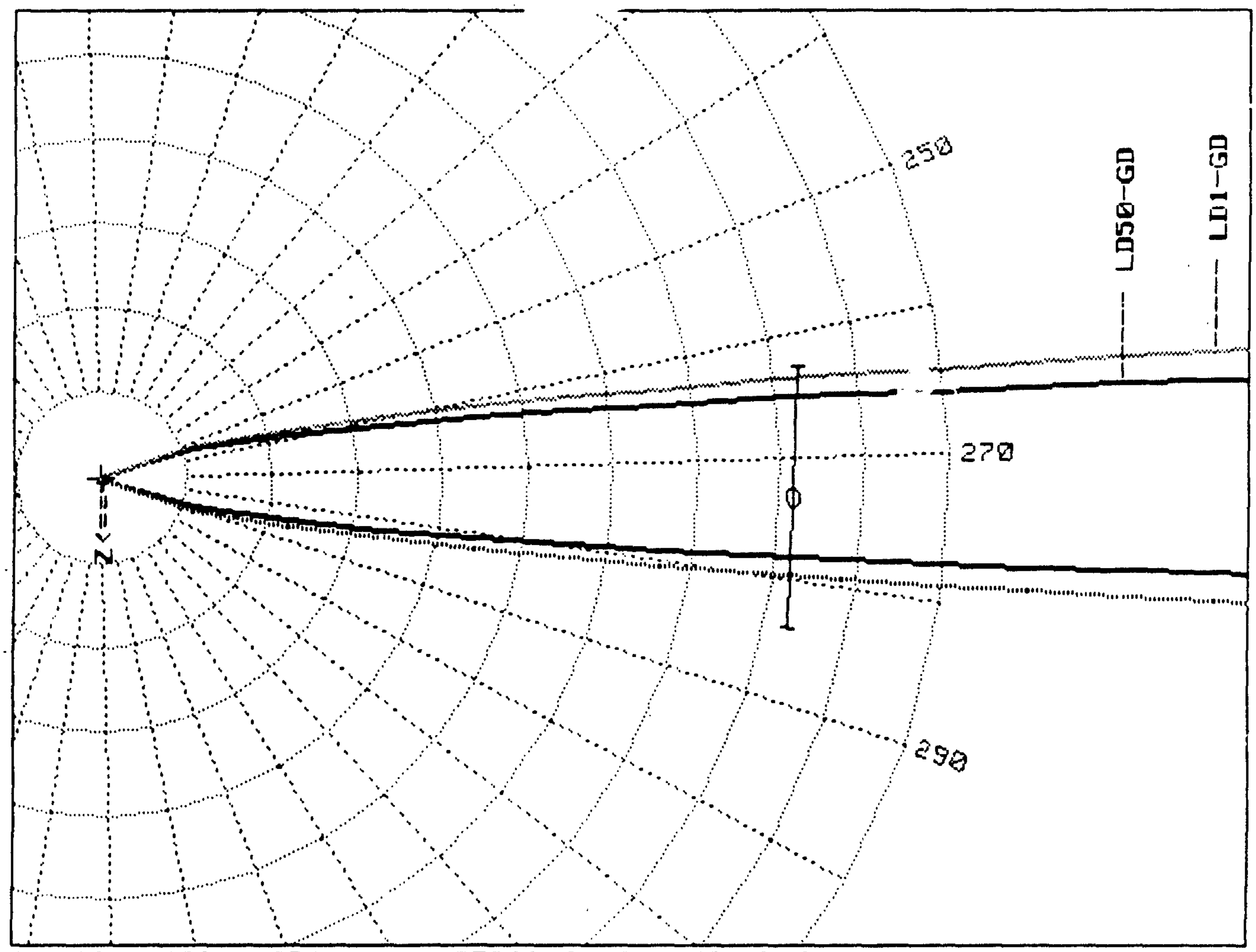
Fig. 2.2

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 500 YARDS BEARINGS IN DEG TRUE PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	5.82750582751 KTS FROM 91.6333333333 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	26109 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	73468 YARDS

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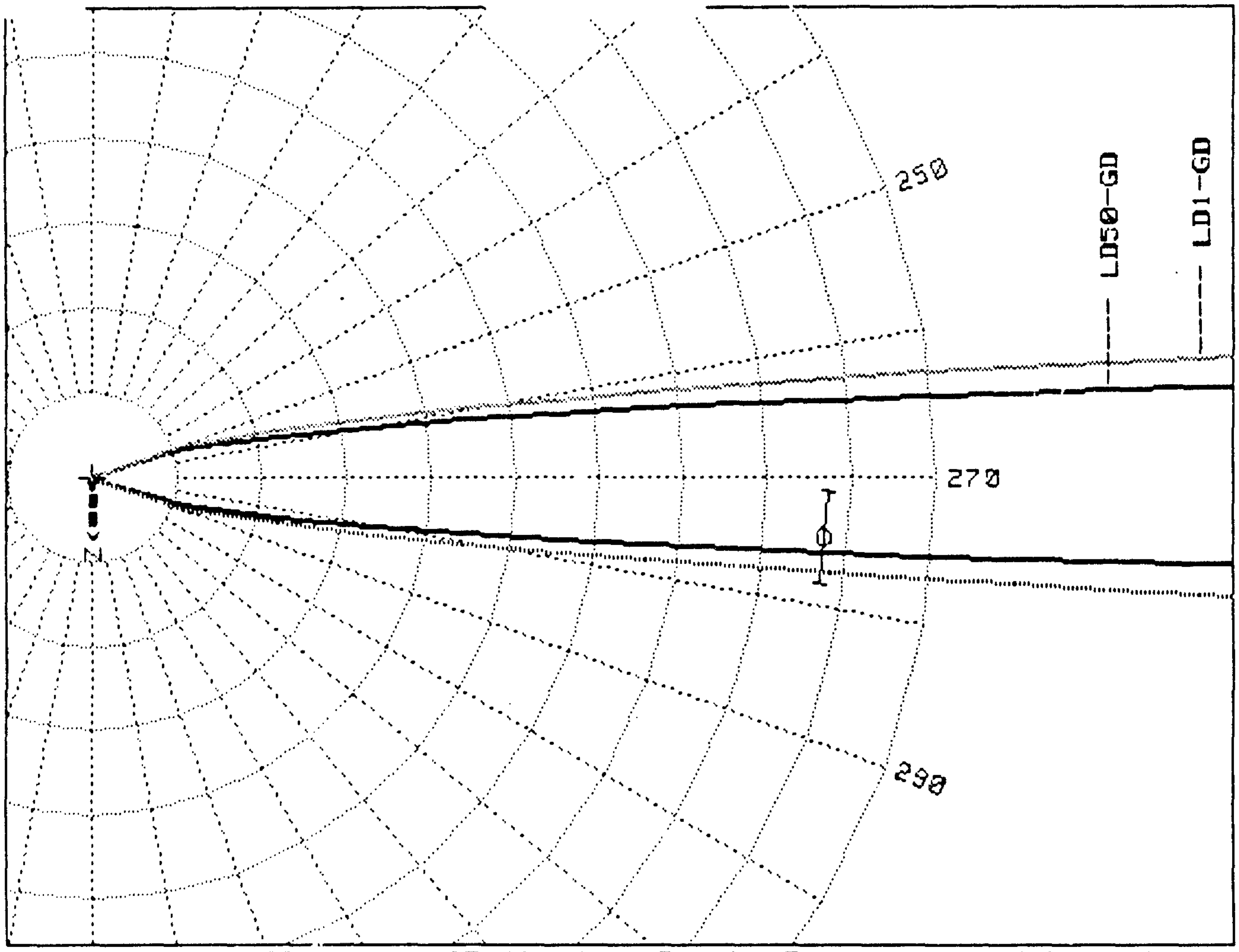
Fig. 2.3

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 500 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	7.77000777001 KTS FROM 89.9333333333 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	21065 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	59274 YARDS

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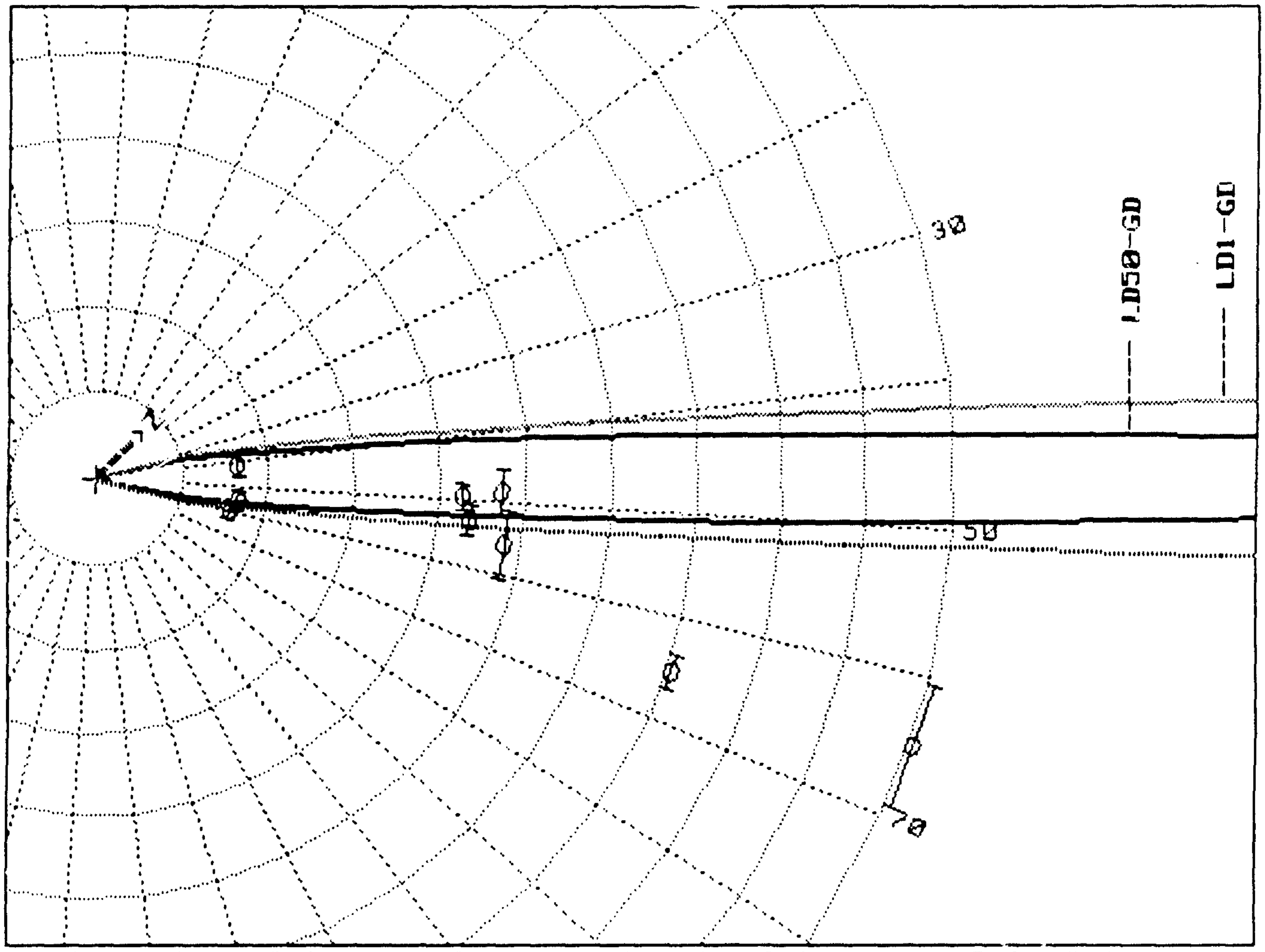
Fig. 2.4

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

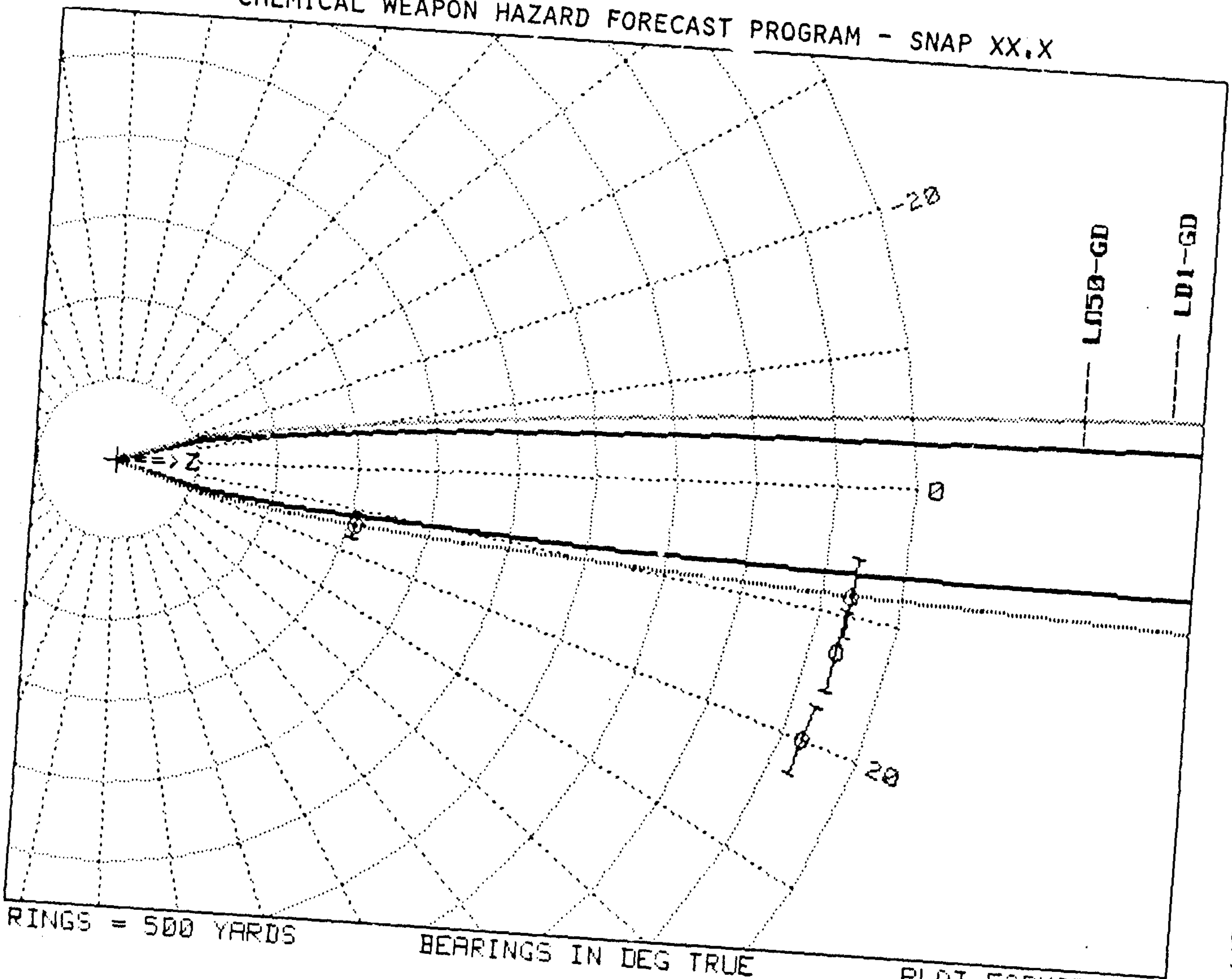
TERRAIN TYPE	OPEN-SEA
MEAN WIND	9.71250971^51 KTS FROM 226.545454545 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

===

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	17833 YARDS
	1% DEATHS - MANY INCAPACITATED	50181 YARDS

Fig. 2.5

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 500 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA	
MEAN WIND	11.655011655 KTS	FROM 181.566666667 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL	
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)	
SOURCE TYPE	POINT-BURST	
SOURCE SIZE (*effective*)	.189 KG	
SOURCE RATE	INSTANTANEOUS	

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	15565 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	43798 YARDS

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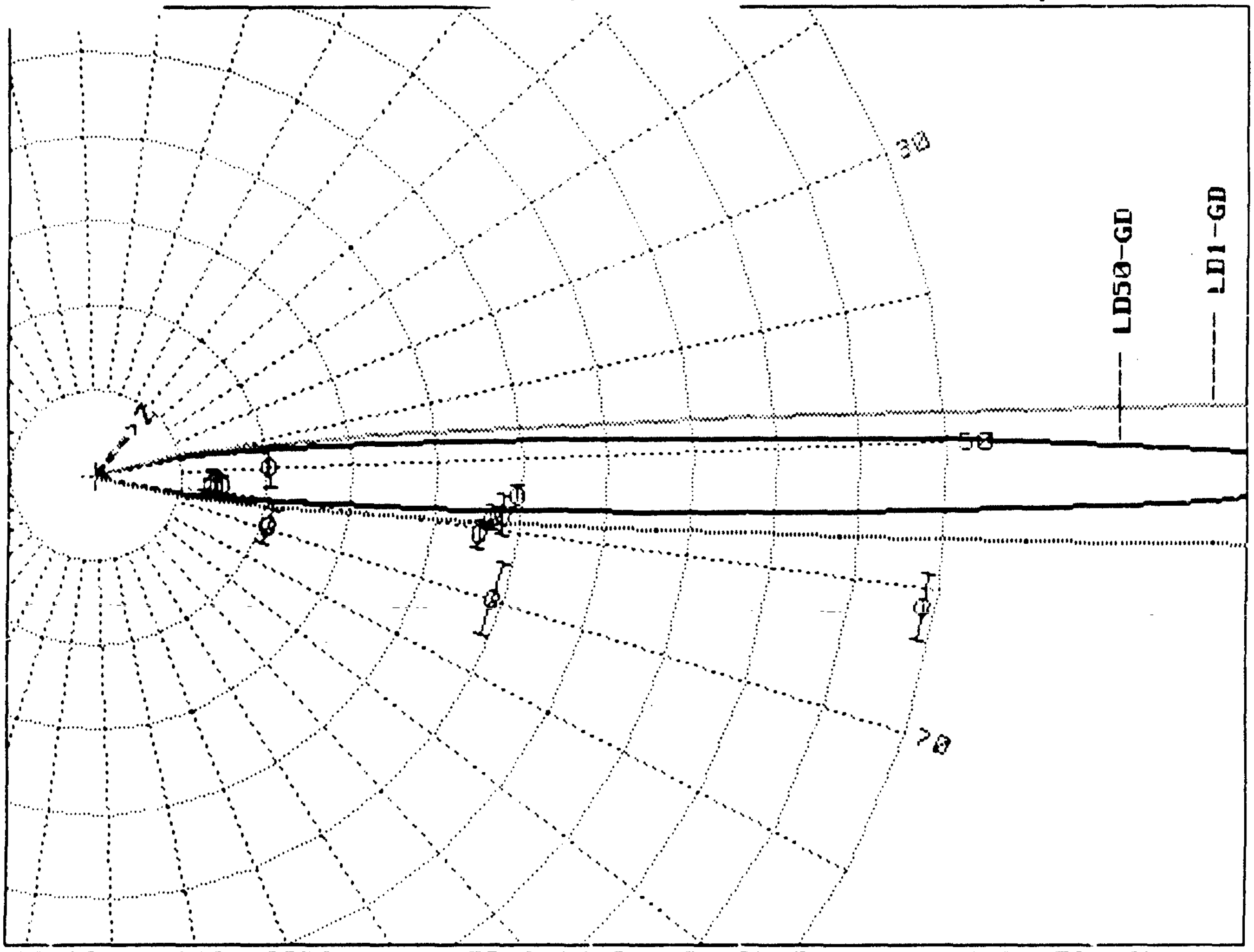
Fig. 2.6

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	13.5975135975 KTS FROM 232.230769231 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	13873 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	39038 YARDS

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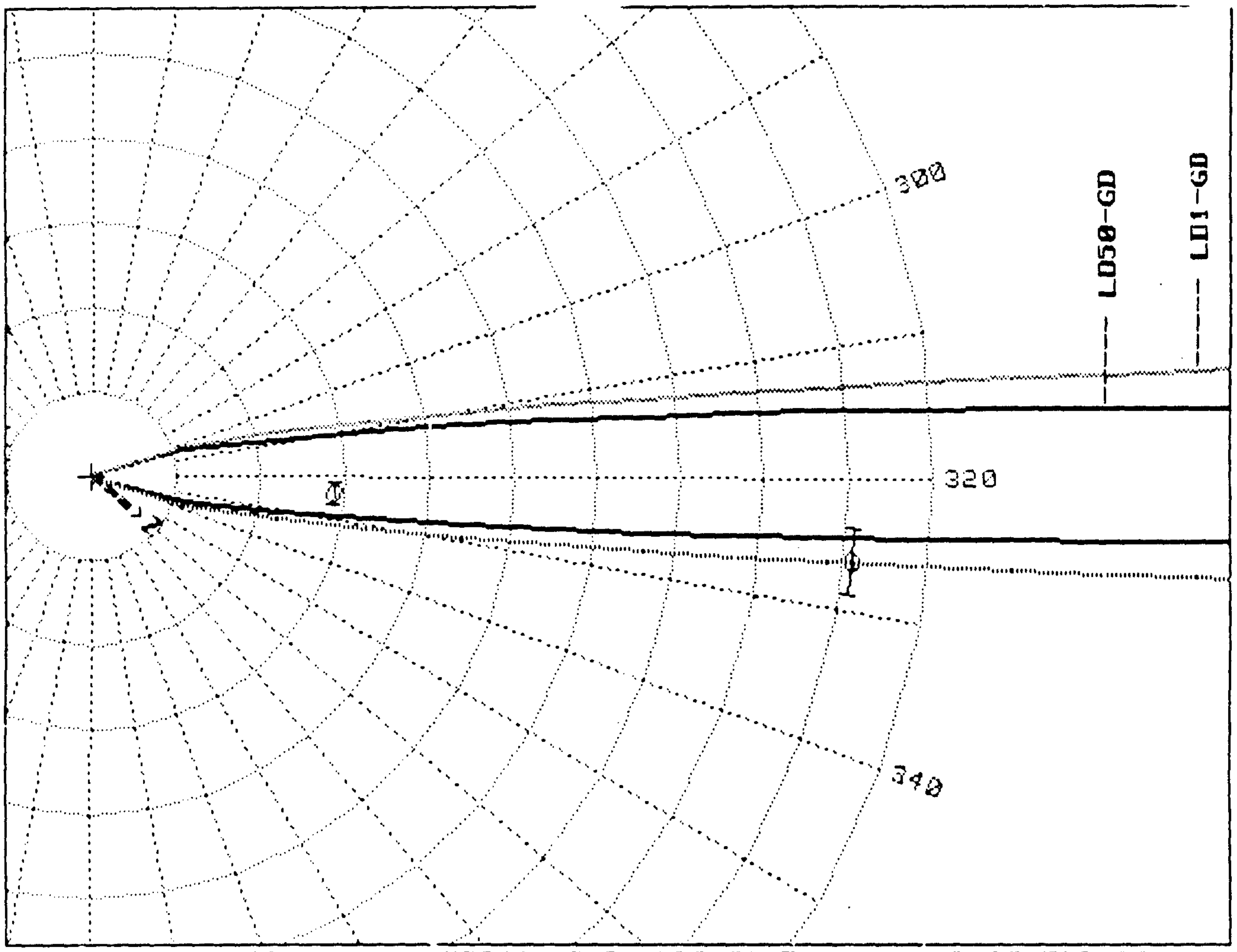
Fig. 2.7

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 500 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	15.54001554 KTS FROM 139.725 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	12557 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	35335 YARDS

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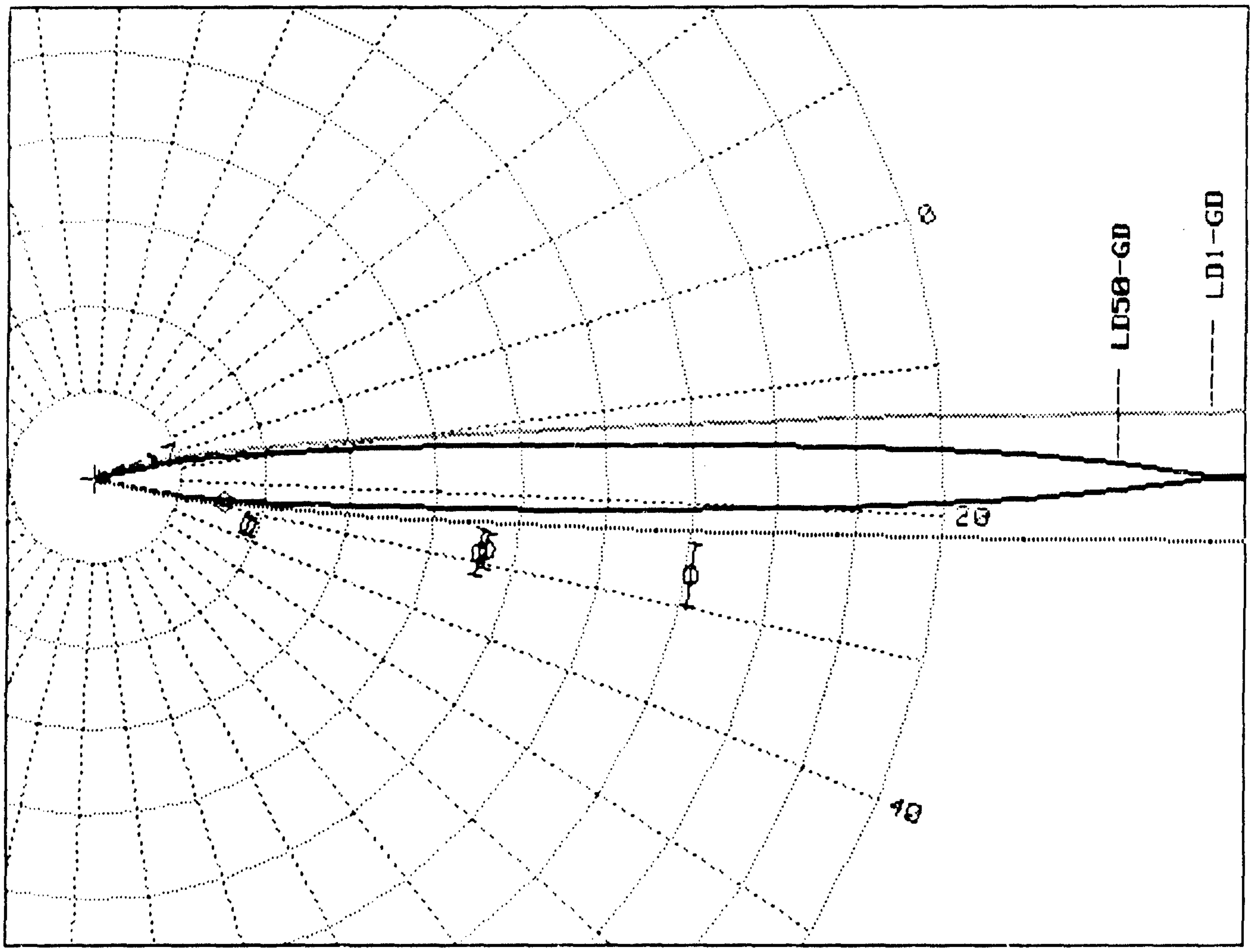
Fig. 2.8

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 1000 YARDS BEARINGS IN DEG TRUE PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	17.4825174825 KTS FROM 197.442857143 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	11501 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	32362 YARDS

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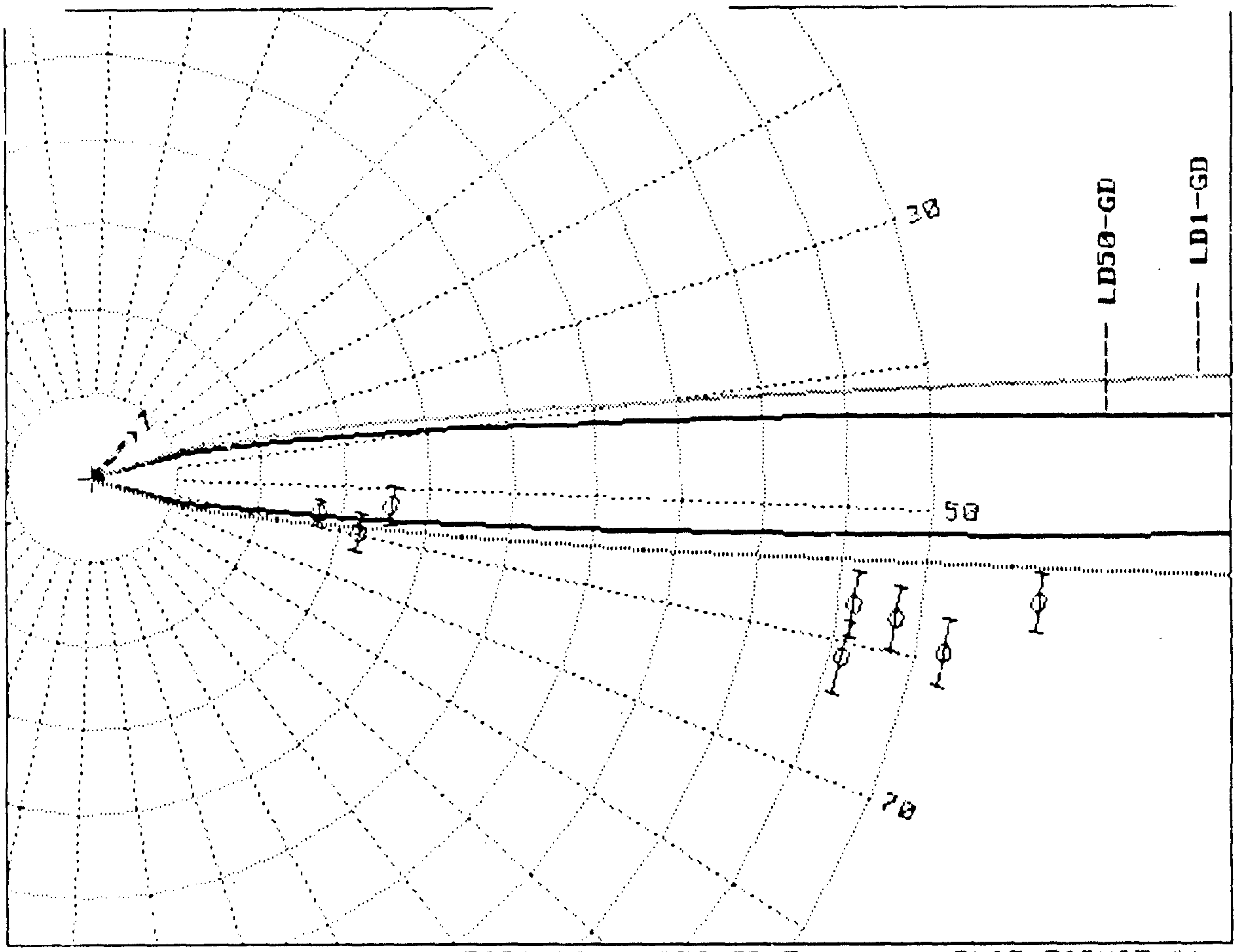
Fig. 2.9

CHEMICAL WEAPON HAZARD FORECAST PROGRAM - SNAP XX.X



RINGS = 500 YARDS   BEARINGS IN DEG TRUE   PLOT FORMAT #1

TERRAIN TYPE	OPEN-SEA
MEAN WIND	19.425019425 KTS FROM 227.565 DEG TRUE
STABILITY CATAGORY	D MODIFIED PASQUILL
MUNITION TYPE	MK116-SIZE BOMB/MISSILE (SCALED)
SOURCE TYPE	POINT-BURST
SOURCE SIZE (effective)	.189 KG
SOURCE RATE	INSTANTANEOUS

==

CONTOUR LABEL (DOSE-AGENT)	POTENTIAL CASUALTY EFFECTS (WITHOUT PROTECTION)	APPROX MAX RANGE
- LD50-GD	50% DEATHS - MOST INCAPACITATED	10631 YARDS
- LD1-GD	1% DEATHS - MANY INCAPACITATED	29915 YARDS

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V. COMPARISON OF THE NPS SIGMA-PARAMETERIZATION .. AN INDEPENDENT DATA SET

This report and the findings of many other investigators have demonstrated that Gaussian-type dispersion model results are heavily influenced by the choice of sigma-y and sigma-z values. Measured values have been shown to fluctuate radically, and are dependent upon numerous independent variables (see Hanna, et al. 1977). Because of this complexity, these investigators (NPS included) inevitably choose to predict sigma via semi-empirical methods. A group of "important" variables are selected, and curve-fitting ensues. Because this approach is based on correlation, and not physical cause-effect relationships, experimental "evidence" should always be required to substantiate results.

To verify the NPS parameterization, the results of a tracer experiment conducted by the German Military Geophysical Office (GMGO) in the North Sea were obtained. (See Groll, et al. 1983). This experiment was performed about 80 km NW of Helgoland, far removed from possible shoreline effects. Sigma formulae presented in this section are based on continuous releases of SF6 gas. Techniques were similar to those used by NPS.

The stability class parameterization scheme selected by GMGO was based on the same two key variables used in the NPS scheme; mean wind speed and air-sea temperature difference. NPS also used relative humidity, but its affect on stability is minor.

The GMGO class boundaries were chosen empirically so that sigma curves would present marked differences. The stability classes are therefore unique, and will not coincide with the NPS/Pasquill-Gifford categories. Some conclusions can be made by interpolation, and noting that the selected independent variables are similar. The neutral classes, centered about negligible air-sea temperature difference or due to high wind speed, should theoretically be identical.

Another problem in comparing the NPS results to the GMGO results was the averaging time. NPS performed one-hour averages in contrast to the two hour period used by the German investigators. This difference should be significant in the sigma-y results, where meander effects are strongly a function of averaging time. Sigma-z, on the other hand, should not be affected by different averaging times for a sampling period larger than a few minutes.

GMGO calculates two separate horizontal parameters; one accounting for meander effects, and another affected only by dispersion relative to the plume centerline (the instantaneous, or puff, sigma-y of the previous section). The two-hour average results presented represent the combined effects of both parameters. At the time of this report, NPS has not converted its instantaneous data set into analytical formulae, so it is not possible to compare NPS and GMGO instantaneous results.

The basic equation used in CWH for the sigma parameterization, a form of which was given in Equ 6, is

$$\sigma(x) = \sigma_{ref} \left(\frac{x}{x_{ref}}\right)^{\alpha} \tag{8}$$

where $\sigma(x)$ is either $\sigma_y(x)$ or $\sigma_z(x)$

σ_{ref} is a constant defining the cloud size at the range x_{ref}

x_{ref} = 100 m

α is an empirical constant

Note that the reference terms can be combined into one constant. The NPS and GMGO constant values used for this comparison are given in the following table.

DATA	STABILITY*	SIGMA-Y α	SIGMA-Y σ_{ref}	SIGMA-Z α	SIGMA-Z σ_{ref}
NPS 1 hr. average	C	.70	20.0	.70	8.0
	D	.69	15.1	.65	3.2
	E	.65	16.1	.62	1.8
GMGO 2 hr. average	2a	.7	39.8	---	---
	2b	.7	27.8	---	---
	6a	.7	39.2	---	---
	6b	.7	27.0	---	---
GMGO "instantaneous"	2	.7	9.7	.56	18.2
	4	.7	8.1	.44	14.9
	6	.7	6.8	.32	12.1

* NPS classes are Pasquill-Gifford equivalent.

GMGO classes are 2: $(\Delta T/U)^2 = [-.3, -.15]$

4: " $= [-.01, .01]$

6: " $= [.15, .3]$

a: wind speed < 10 kts

b: wind speed $\geq$ 10 kts

where ΔT is air-sea temperature difference (K)

U is mean wind speed (m/s)

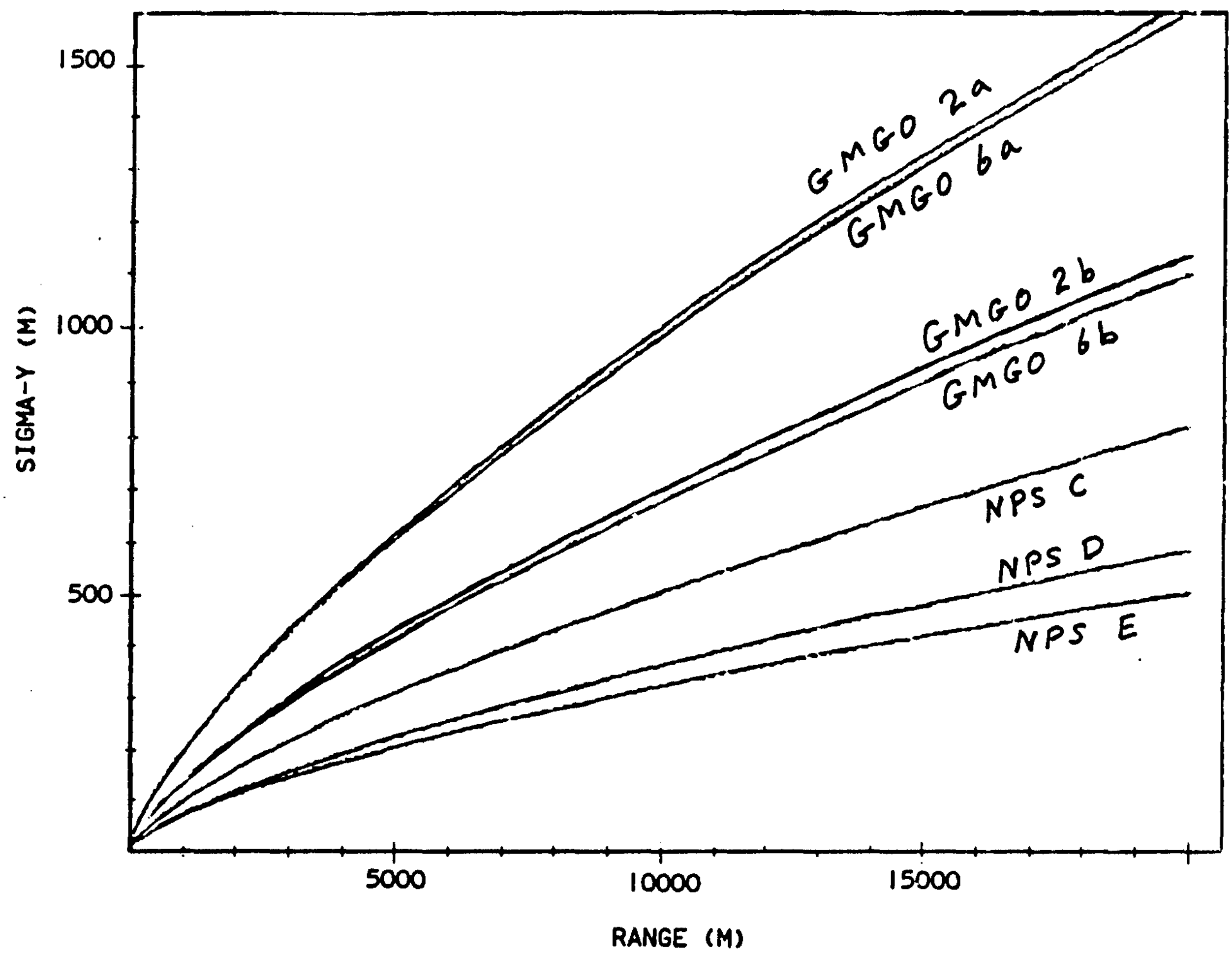

Figure 3.1. Sigma-y vs. range for the Naval Postgraduate School 1-hour average scheme and the German Military Geophysical Office 2-hour average scheme. The GMGO class 2 and NPS class C are unstable data, while the GMGO class 6 and NPS class E are stable. NPS class D is neutral stability. GMGO class 4 representing neutral conditions was roughly in between the class 2 and 6 curves. Subscript "a" refers to low wind speeds, while "b" references high speeds.

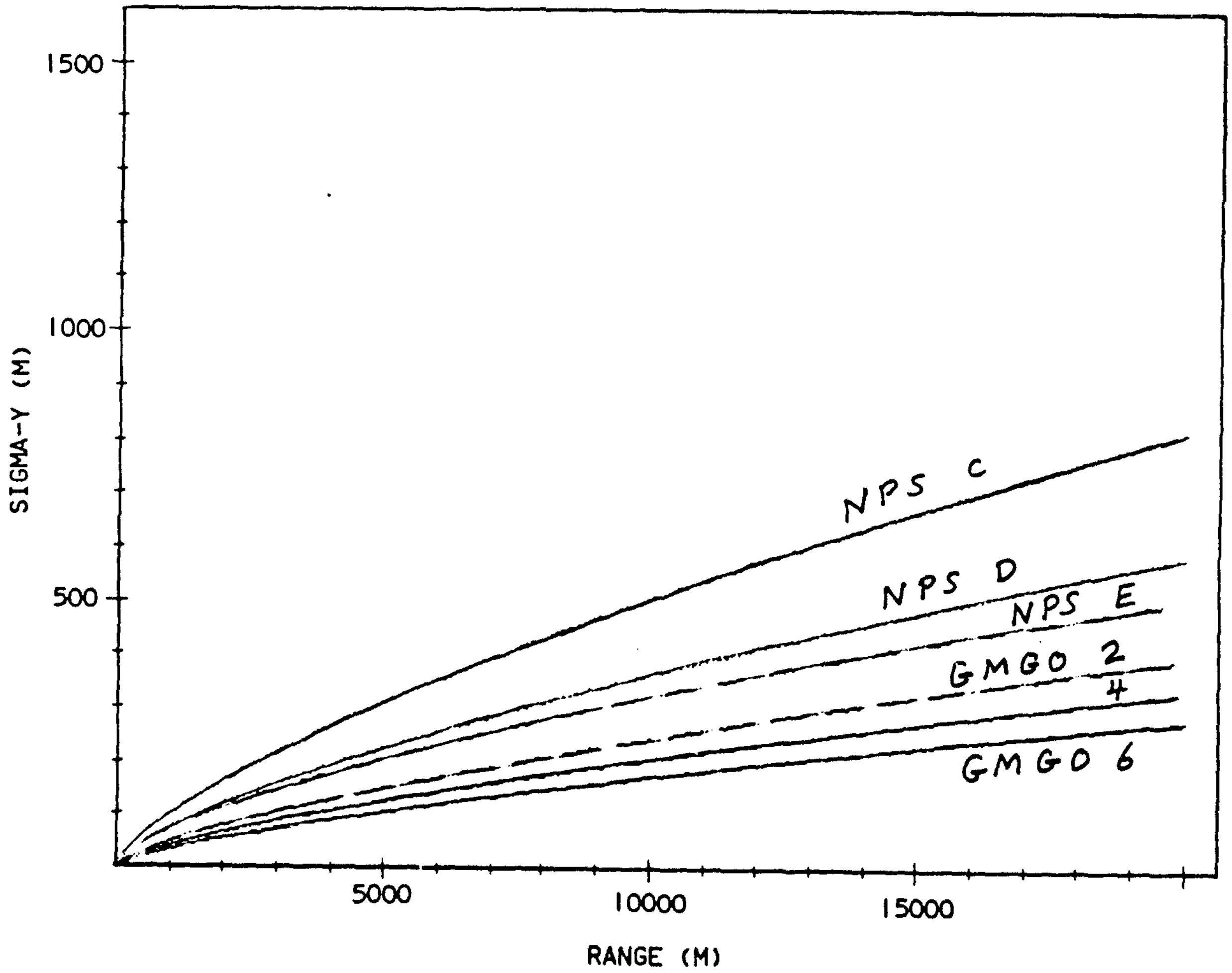

Figure 3.2. Sigma-y vs. range comparison between the NPS 1-hour average scheme and the GMGO "instantaneous" data set (representing dispersion from the center of mass).

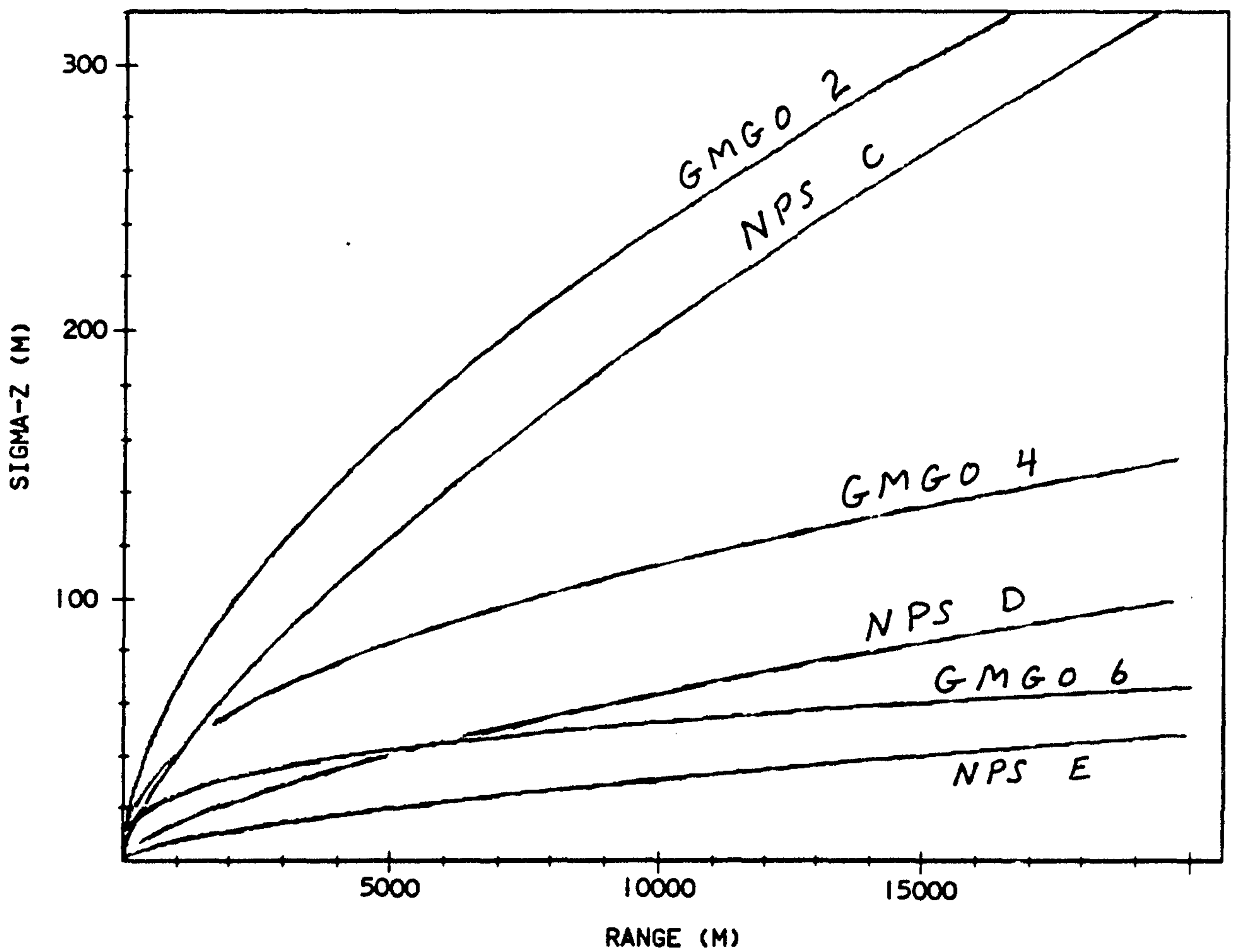

Figure 4. Sigma-z vs. range comparison between the NPS 1-hour average scheme and the GMGO 2-hour average scheme. NPS class D and GMGO class 4 should ideally compare directly. Other classes should not be considered as "matched pairs".

Figure 3.1 compares the GMGO 2-hour average sigma-y to the NPS 1-hour averages. Figure 3.2 compares the GMGO instantaneous values to those same NPS 1-hour averages. The figures show the NPS curves to lie, as expected between the GMGO 2-hour and instantaneous curves.

The first conclusion one can draw from the figures is that meander dominates the results. This can be seen from the large differences in the results for the various averaging times: instantaneous, one-hour, and two-hour. All of the sigma-y curves are bounded by the GMGO two-hour, 2a curve on one side and the GMGO instantaneous, 6 on the other.

Figure 3.1 shows the importance of the GMGO wind speed subclass. Classes 2a and 6a, and also 2b and 6b, lie almost on top of each other, while the a and b curves show large differences in their behavior. Recall from the table that subclass a is for wind speed less than 10 kts while b is for 10 kts and greater. This result is not conclusive since wind speed is one parameter needed to determine stability and cannot be treated as a completely independent parameter. However, the results do indicate that including wind speed only in the stability calculation probably does not sufficiently account for the dependence on this parameter. This may be due to the strong wind speed dependence of meander. The GMGO instantaneous results presented in Figure 3.2 are essentially meander independent and do not show the strong wind speed dependence.

One would expect that the GMGO and NPS neutral classes would show the same behavior. The figures show that this is not the

case. (Note that the neutral GMGO case is not shown in Figure 3.1 in order to reduce clutter on the graph. The results fall between those for classes 2 and 6.) This is not of much concern since the two analyses are not directly comparable because of the different averaging times, class definitions, etc.

Figure 4 shows the comparison of sigma-z values. It is apparent that the GMGO values are somewhat larger than the NPS, but the agreement is generally better than for sigma-y. The most significant fact is that a stability classification scheme accounts for the variability in vertical diffusion much better than it does for horizontal, cross wind diffusion. This is due to the fact that meander does not contribute to vertical diffusion.

No in-depth analysis of the comparison of NPS and GMGO results has been undertaken. The purpose of this comparison is only to show verification (or lack of verification) of the CWH model predictions. NPS preliminarily concludes that the empirical methods for determining dispersion are similar, but do not sufficiently agree to conclude that either parameterization fully explains dispersion. Uncertainties could be calculated and errors estimated, but adding such estimates to the already empirical formulae would give confusing and difficult to interpret results. In order to proceed further with the comparison it would be necessary to reanalyse one of the data sets based on the classification scheme used for the other.

CONCLUSIONS

Comparison of SNAP's Chemical Weapons Hazard Program to the one-hour average plume dispersion data used in its parameterization has shown the model is operating as expected. When drift of the cloud (due to meander) is included, the region of impact is shown to dramatically increase.

In its present form, CWH appears to be predicting a hazard "envelope" that is reasonable when examining a possible puff event, taking meander effects into consideration. The downwind axis ranges predicted by CWH to be hazardous are undoubtedly underestimated, since the range-dependent sigma-y values are approximately the upper limit of the pseudo-instantaneous puff widths.

The NPS sigma formulae are reasonably close to the results of an independent tracer experimen' .llowing CWH to be considered as a site-independent model. The comparison does point out some differences, however, and future research should examine refinement of stability parameterization schemes. It is becoming apparent that stability is a good parameter for predicting vertical diffusion but is not sufficient for horizontal diffusion.

To improve sigma parameterizations, and ultimately CWH's usefullness to SNAP, meander effects must be directly addressed. This could mean a different "concept" in the prediction of hazard regions is needed. The problem can be divided into two predictions; one predicting the characteristics of a single puff in its center of mass coordinate system, and a second predicting

the probablistic characteristics of the puff's downwind trajectory.

CWH is a single parameter diffusion model: It assumes that the hazard moves in the downwind direction and uses puff/plume width to predict the width of the hazardous corridor. This type of model works well for continuous plumes and long averaging time. It will also work for burst releases if the prediction required is the total area over which a hazard might occur. In that case, as has been stated above, the downwind hazard distance has been underestimated. This could be corrected by using the puff relative diffusion width to determine the distance.

The problem with this "patchwork" approach is that it lumps together two entirely different concepts. One is that the spread of the puff about its center of mass reduces its lethality. The second concept is that the puff may or may not pass over a given location. It is important at this state of the CWH model development to be able to correctly predict both effects. Exactly how the results will be used depends on user needs, and it may be that more than one type of CWH display is needed. In any event, an investigation of meander should be undertaken so that the probability distribution function for the puff center of mass location will be known.

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3. Skupniewicz, C.W. and G.E. Schacher (1984): Measured Plume Dispersion Parameters over Water. NPS-61-84-012.

4. Schacher, G.E., C.W. Fairall and P. Zanetti (1982) "Comparison of Stability Classification Methods for Parameterizing Coastal Overwater Diffusion", Proc. 1st Inter. Conf. on Meteorology and Air/Sea Interaction of the Coastal Zone, AMS, p 91.

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